Computer simulation of the growth of heterostructure systems

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We have investigated the growth of heterostructures with high lattice mismatch and the growth of quantum wires on the top of ridges and through shadowing masks. Simulations are performed within a Monte Carlo scheme using tetrahedral lattice structure of semiconductor materials. It is shown that results of different simulations present similarities that we attribute to the primary role of kinetic effects as the driving force during epitaxial growth. The formation of 3D islands showing (111) facets, or (111) side walls when depositing through a shadowing mask, has been observed. The facets are of better quality than the top (001) surface because of the higher mobility of atoms on these facets. © 1997 Elsevier Science Ltd.

1. Introduction

Molecular Beam Epitaxial (MBE) growth of heterostructure systems can now be performed, while a decade ago only homoepi-

taxial growth of good quality was possible. The reason is that improvements in technology processes have allowed a better control of strain and stress in the deposited layer. A variety of problems still remain unsolved, which need a better understanding of basic physical mechanisms involved during the process. Patterning of the (001) oriented GaAs substrates with grooves and ridges has been extensively studied experimentally [1–4]. MBE growth of GaAs, AlAs and AlGaAs on V-grooved GaAs substrates was investigated. V-grooves were aligned along the [110] direction on (001) GaAs substrates and had V-shaped profiles with (111)A side walls due to the anisotropic etchings. By using the effect of different growth behavior of GaAs, AlAs and AlGaAs, multiple crescent-shaped GaAs quantum wires, with a size of about (140–160 A) × (400–500 A), were successfuly grown at the bottom of the V-grooves [5, 6]. Facetted

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growth of GaAs/AlGaAs epilayers on ridges has been studied in Refs [7,8]. Rectangular ridges aligned along [110] direction on (001) surface were formed through a photoresist mask by reactive ion etching, and AlGaAs layers were regrown on them by MBE. (111)B planes on both sides of the ridge as well as the (001) facets in the center of the ridge were formed. With decreasing ridge width, the (111)B planes restrict the formation of (001) facets on top of the ridges resulting in triangular shaped structures. In this way, the quantum wires were grown in Ref. [7].

Similar effects have been observed in strained systems where the roughening of the growing layer is reported in a variety of cases including IV–IV [9,10], III–V [11–14], and II–VI [15] compounds or their combinations [16,17]. The roughening occurs after a few monolayers deposition and may lead to the formation of three-dimensional islands exhibiting (111) facets. The morphology of the surface is very close to the structure of films deposited on the top of ridges and through shadowing masks. This is not surprising since it is known, from elasticity theory, that the strain in flat layers is at the origin of topological instabilities [18], which can lead to the formation of ridges.

The aim of this paper is to go beyond energetic considerations by taking into account the kinetic effects through a Monte Carlo simulation. Indeed, in an MBE experiment, the growing layer is never in its thermodynamic equilibrium state. The various migration rates govern geometrical aspects of the layer and it is important to check to what extent the results of the thermodynamic models remain valid under the real experimental conditions. In Section 2, we investigate the initial stages of the growth of highly strained layers to show the roughening of the surface and the facetting of the 3D islands formed. Section 3 is devoted to the study of homoepitaxial growth on patterned substrates, with surfaces presenting ridges or covered by masks, leading to quantum

wire structures. We will show that facetting can also occur by deposition through masks. Furthermore, once the facets are formed, as is the case in the deposition on the top of ridges, configurations similar to those obtained in heteroepitaxial growth with high lattice mismatch may occur. Results of the two models are compared and discussed in Section 4.

2. Growth of strained layers

Our simulation model is an SOS model based on the tetrahedral lattice structure of semiconductor materials. Four kinetic processes: deposition of atoms on the surface, the intralayer and interlayer migrations of atoms and the evaporation from the surface, are taken into account. The simulation procedure follows a Monte Carlo scheme where we attribute a time to each possible single atomic event in the layer, using the Arrhenius law to determine the probability of the event. We then assume that the event corresponding to the minimum time will occur. In order to simulate the strain effects, we have assumed that the various activation energy barriers used in the Arrhenius law are composed of a chemical energy term, derived from the broken bond energies, lowered by the atomic strain energy. This strain energy is calculated in the equilibrium configuration of the atoms within the layer. It leads to an acceleration of the motion of the most stressed atoms and to a relaxation of the deposited layer. We have calculated the strain energy within an elastic model using a Valence Force Field approximation [19]. The strain energy is expressed in terms of bond elongations and bond angle variations, using a simplified Stillinger–Weber type potential [20,21]. Elastic constants of GaAs are used to simulate III–V semiconductor materials. The equilibrium atomic configuration is found by the minimization of the total strain energy with respect to atomic positions. The minimization is performed after each single atomic event, using the Newton–Raphson method wich allows an optimization of the computing time.

Simulations are carried out at 700 K, using 30×30 atoms substrates with periodic boundary conditions. A lattice mismatch of 8% between the substrate and the layer is assumed. The high lattice mismatch reduces the size of the observed islands and therefore allows the use of relatively small substrate sizes. The morphology of the growing layer is shown in Fig. 1. It can be seen that hills and valleys are present on the surface due to the upward migration of adatoms in highly stressed positions. The hills show a facetted structure with (111) oriented facets. The valleys are oriented in the [110] directions, in agreement with experimental observations.

The (111) orientation of the facets is closely related to the large flux of upward migration of atoms which can only occur on facets with low surface migration energy. The onset of 3D growth can clearly be seen in Fig. 1, and agrees with the mechanism of strain relaxation. This is illustrated in Fig. 2, where the maximum and average relaxation in successive layers are presented. The relaxation is measured by the local strain, calculated with respect to the substrate lattice parameter, and varies from 0 to 8% which is the misfit between the substrate and the layer. It can be observed that the islands are almost completely relaxed after few

monolayers. Some discrepancies between the average and maximum relaxation exist, showing the inhomogeneous relaxation within a given layer. Indeed, calculations show that the maximum relaxation occurs at the island boundaries where the strain energy falls off very rapidly. On the other hand, a few atomic distance away from the boundaries, a constant strain close to the average value is reached. It can be seen in Fig. 2 that the strain is relieved smoothly. It should be noted that the 3D growth mode is the one which allows such a relaxation at the initial stages of the growth. This growth mode can continue further by separation of the already formed islands or change to 2D growth mode by coalescence of these islands and the formation of misfit dislocations at the boundaries between them.

3. Growth of quantum wires

Simulations of homoepitaxial growth of Si on Si(001) substrates have been carried out in basically identical experimental conditions to the case of heteroepitaxial growth in Section 2. The substrate is, however, patterned and presents ridges with (111) facets or is covered by the shadowing masks oriented in |110] direction. The goal is to investigate the similarities between homo- and hetero-
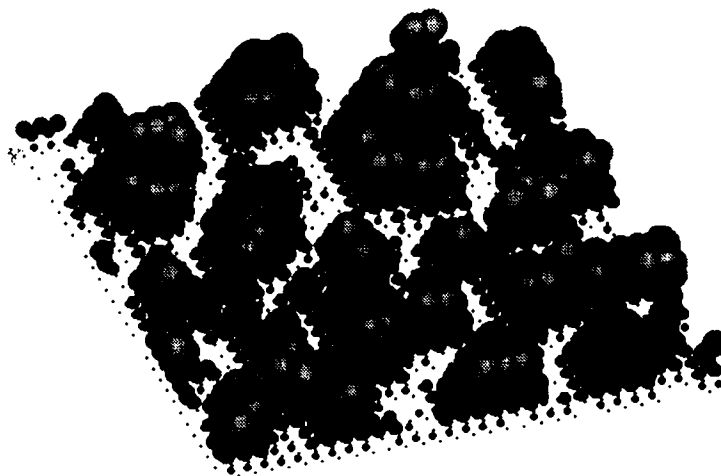

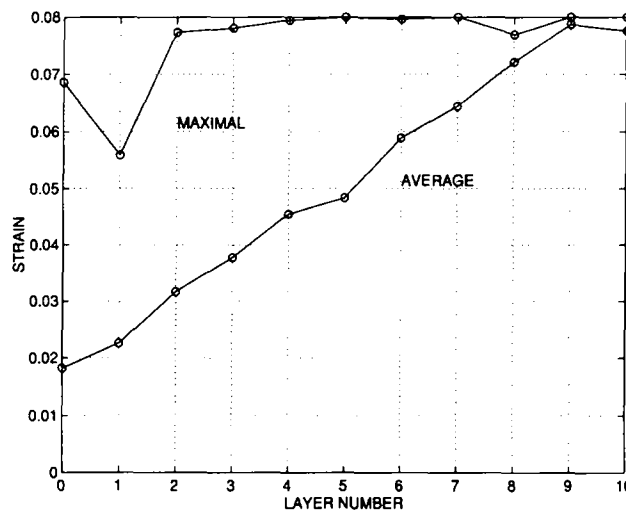Fig. 1. Perspective view showing the morphology of a portion of the growing layer.

Fig. 2. Average and maximum relaxation in successive layers of the deposited film.

epitaxial growth due to kinetic effects. The substrate was covered by a mask with a 30×80 atoms window, or was made of 40×20 atoms ridges aligned along the [110] direction. Elongated rectangular-shaped substrates are used here to account for the actual geometry of the quantum wires. The deposition rate was 1 monolayer/sec. The four kinetic processes were simulated using the Arrhenius rate equations, taking into account up to second-nearest-neighbor interactions. They are expressed as: $R = R_0 \exp-(n_1E_1+n_2E_2)/kT$, where n_1 and n_2 are, respectively, the numbers of the first and second-nearest neighbors, and E_1 and E_2 are the corresponding interaction energies. The choice of the parameters was based on the experimental data on the growth of Si(001) [22]. According to this, numerical values used in the simulation of migration processes were chosen to be E_1=0.6 eV, E_2=0.1 eV. Energy terms for the evaporation event were taken to be E_1=1.1 eV, E_2=0.2 eV. The pre-exponential hopping rate was assumed to be R_0=10^{13}s^{-1}.

Migration probabilities on the (001) surface are lower than on the (111) surface. That is why, in the first stages of our simulations of the growth of quantum wires on the top of ridges, we have

assumed an infinitely large difference of these rates. Due to this assumption, we obtained flat (111) side walls with clear narrowing of the quantum wire during the growth. The top (001) surface is, however, rough. In Fig. 3, the roughness is plotted versus time, during heteroepitaxial growth of Section 2 (curve a), during the homoepitaxial growth of Si/Si(001) (curve b), and for the (001) surface on the top of ridges (curve c). The overall roughnesses (curves a and b) have similar behavior at the beginning of the growth. Some discrepancies arise later when the island formation starts and where the strain effects are the most important. The two curves tend to join at the end when the islands are formed and kinetic effects become dominant. The surfaces on the tops of ridges present obviously less roughness than the overall layer. The assumption of an infinitely large difference between the migration rates on different planes has been relaxed in the simulation of growth of quantum wires through shadowing masks. Rather, the actual migration rates have been taken into account everywhere in the deposited film. In these simulations, we first deposited five monolayers of Si on Si(001) surface with the dimension of 60×80 atoms. After that, we started the deposition of Si atoms on the central region of
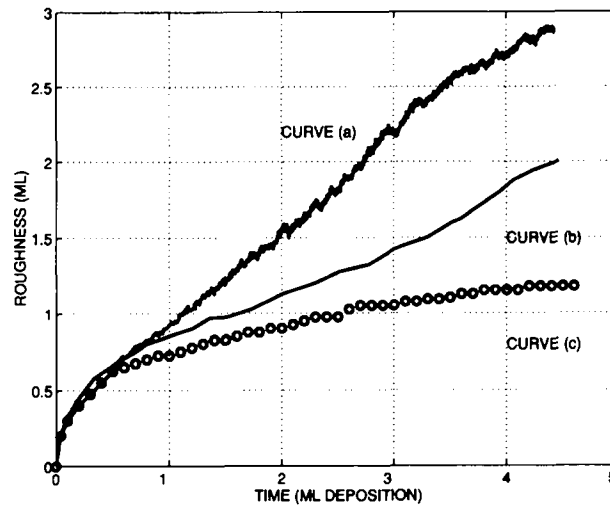
Fig. 3. Roughness of the growing layer versus time (in ML deposition units) during the heteroepitaxial growth of III–V compounds with 8% lattice mismatch (curve a) and during the epitaxial growth of Si on Si(001) (curve b). The roughness of the top (001) surface is also represented (curve c).

30×80 atoms. Figure 4 shows the surface configuration of such a quantum wire after deposition of six additional monolayers on the already five monolayers thick Si(001) buffer layer. The formation of facets with (111) side walls and (001) surface on the top of the structure is also observed. Here, the (111) side walls are not perfectly flat as in the case of growth on the top of ridges, but they are of better quality than the top (001) surface, as can be seen on Fig. 4. Again, the morphology of the top surface is similar to the case of heteroepitaxial growth, presented in Fig. 1.
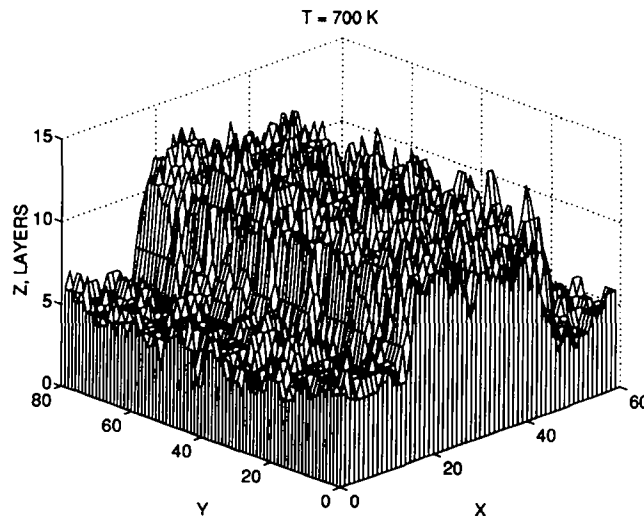

Fig. 4. Surface configuration of a quantum wire deposited through a rectangular shadowing mask.

4. Conclusion

We have performed simulations of homo- and heteroepitaxial growth to investigate kinetic mechanisms and compare their effects with those of models derived from thermodynamic equilibrium considerations. It is shown that some features of the growth are similar in both cases, although large elastic strains are present in the case of heteroepitaxial growth with lattice mismatches as large as 8%, while they are completely absent in homoepitaxial growth. In particular, the morphology of the surfaces showing (111) facets has been observed in both cases with comparable roughness evolution during the deposition. Further, the lattice relaxation and 3D growth mode have been shown to occur in heteroepitaxial growth with high lattice mismatch. The kinetic effects can be best observed if their temperature dependence is studied, but these results have not been introduced here to keep within the allowed space. Finally, it is possible to merge the two simulations to investigate the growth of SiGe/Si quantum wires with moderate lattice misamatch. Indeed, after the deposition of the buffer layer, as described in Section 3, we can start the deposition of Ge atoms, or a simultaneous deposition of Ge and Si atoms, to grow SiGe/Si layers.

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