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Surface orientation influence on the characteristics of GaAs substrates high-temperature annealing

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Abstract. Dependencies of congruent evaporation temperature T_c and desorption activation energies of GaAs components on the substrate surface orientation are analyzed using Monte Carlo simulation. On the vicinal surfaces with the (111)A orientation at temperatures exceeding T_c, metal droplets start to grow at step edges and with the (111)B orientation droplets nucleated randomly on the terraces. The droplet concentration on the (111)B surface is higher than that on the (111)A. The droplet-crystal interface roughness is different for the (111)A and (111)B orientations. T_c of (111)B surfaces is lower than that of (111)A surfaces. For both surface orientations, T_c decreases when the terrace width of the vicinal surface is lower than the double gallium diffusion length. The dependence of gallium and arsenic desorption activation energies on the vicinal surface misorientation is demonstrated. A sharp increase in the arsenic desorption rate is observed with an increase of the (111)A surface coating with liquid gallium.

1. Introduction

Different volatilities of $A^{III}B^{V}$ semiconductor components result in the surface roughening and metal droplets formation during high-temperature annealing. It was demonstrated experimentally that the congruent Langmuir evaporation temperature depends on the surface orientation [1, 2]. Up-to-date there has been no detailed theoretical description of this phenomenon. Monte Carlo (MC) simulation is the technique that allows analyzing surface morphological transformations at the atomic level. The examination of surface orientation influence on the main characteristics of $A^{III}B^{V}$ substrates Langmuir evaporation is fulfilled in this work by the MC simulation.

2. Monte Carlo model

The simulation is carried out using the program package SilSim3D on the base of kinetic lattice MC model [3]. The MC model of GaAs semiconductor Langmuir evaporation is close to the droplet epitaxial model [4]. Its main feature is a possibility to imitate the liquid phase in the lattice model. The basic processes considered in the model are: molecular arsenic creation and dissociation, gallium melting and crystallization, GaAs dissolution in liquid gallium, metal and arsenic atoms diffusion, As_2 diffusion, gallium evaporation in the atomic Ga form and arsenic evaporation in the molecular As_2 form. The probability of each event is determined by its activation energy. These energies are the model input parameters model. The details of MC model realization and the chioce of the energy parameters can be found elsewhere [4, 5].

3. Results and discussions

The simulations were fulfilled on the vicinal GaAs substrates with (111)A and (111)B surface orientations in the temperature range of 800 – 1200 K. At temperatures lower than congruent evaporation temperature T_c, the layer-by-layer evaporation was observed at equal arsenic and gallium evaporation rates. At $T > T_c$ liquid metal droplets are created on the surface. On the (111)B surface the droplets are formed chaotically over the whole substrate surface and, on (111)A, the drops nucleation starts near the steps (Fig. 1a,b). The Ga droplets concentration is appreciably higher on the (111)B surface than on the (111)A surface. The model value T_c for the (111)A orientation is higher than that for (111)B according to the experimental data. The droplet-crystal interface roughness is different for the (111)A and (111)B surfaces. For the GaAs(111)B the interface is practically flat and, for GaAs(111)A, the interface roughness evolves. The difference in the droplet-substrate interfaces on the (111)A and (111)B surfaces is preserved at high temperatures. The cross-sections and a top view of the GaAs (111)A and (111)B model substrates after the annealing at T = 1000 K and T = 1200 K are shown in Fig. 1.

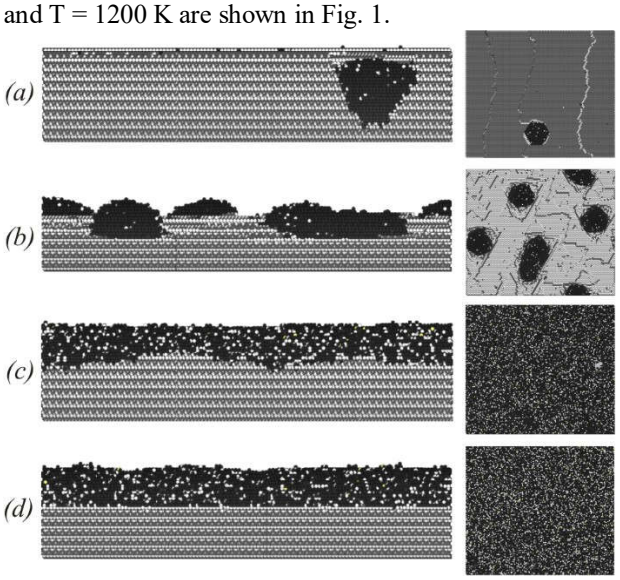

Fig. 1. *Cross-sections and top views of GaAs model substrates (111)A (a, c) and (111)B (b, d) after the annealing at T = 1000 K (a, b), T = 1200 K (c, d). Liquid gallium is marked in black, solid Ga – in gray, As – in white colors.*

Separate Ga drops are created on the surface at $T = 1000$ K. At $T = 1200$ K the substrates are completely covered by a liquid gallium layer. A smooth droplet-substrate interface is preserved on the GaAs(111)B surface and, on GaAs(111)A, the interface roughness is developing. This is due to the GaAs etching rate dependence on the surface orientation: the (111)A surfaces are etched with liquid gallium more actively than (111)B. The simulation revealed that congruent evaporation temperature T_c, Ga and As_2 desorption activation energies E_{des} depend on the

vicinal surface misorientation that is on terrace width L. The L decrease results in T_c lowering and E_{des} increase. These values cease to change when L exceeds the gallium diffusion length before evaporation. A comparison of the model values of T_c and E_{des} with the experiment ones is presented in Table 1. The L increase from 20 nm to 360 nm leads to an equality of gallium E_{des} values in the model and experiment, and approach of the model arsenic E_{des} values to the experimental ones. The L influence on the T_c value is more pronounced for the (111)A surface. It is worth noting that the model T_c value on the (111)A surface for L = 360 nm is higher than the experimental one. This discrepancy may be due to the model substrate perfection. T_c decreases when introducing the point defects on the (111)A surface. T_c for the (111)B surface is insensitive to the point defects concentration. This difference can be explained by different volatilities of gallium and arsenic. On the ideal (111)B surface the high point defects concentration is created spontaneously during the initial stage of annealing, and an additional defects introduction does not change the characteristics of Langmuir evaporation.

Table I. *Main parameters of GaAs Langmuir evaporation*

Parameter	Simulation	Experiment
T_c, *K* *(111)A*	930 (L = 20 nm) 1000 (L = 360 nm)	950 [1] 930 [2]
T_c, *K* *(111)B*	890 (L = 20 nm) 900 (L = 360 nm)	900 [1] 890 [2]
E_{des}*(Ga), eV* *(111)A*	2.52 (L = 20 nm) 2.50 (L = 360 nm)	2.5 [1]
E_{des}*(Ga), eV* *(111)B*	2.50 (L = 20 nm) 2.47 (L = 360 nm)	2.4 [1]
$E_{des}(As_2)$*,eV* *(111)A*	3.37 (L = 20 nm) 3.21 (L = 360 nm)	3.0 [1]
$E_{des}(As_2)$*,eV* *(111)B*	3.84 (L = 20 nm) 3.25 (L = 360 nm)	3.2 [1]

For the GaAs(111)A surface at some definite temperatures T*, the arsenic evaporation rate temperature dependence demonstrates a change in the E_{des}. This phenomenon is also due to different etching rates of (111)A and (111)B surfaces. The temperature dependence of evaporating As to the Ga fluxes ratio is shown for two surface orientations in Fig. 3(a), and in Fig. 3(b) – for two L values. At $T > T_c$ this ratio > 1. For temperatures lower than some critical value T*, the As evaporation increases more intensively on the (111)B surface than on (111)A, since the upper GaAs(111)B layer consists of arsenic atoms, and As is more volatile than Ga. However, with the temperature rise, the surface part covered with liquid gallium increases. It was demonstrated in [6] that the GaAs evaporation rate increases when the GaAs surface is covered with liquid gallium. So liquid gallium acts as a pump. At $T = T$* the fluxes, evaporating from the GaAs(111)A and GaAs(111)B substrates, are equal. At $T > T$*, when an appreciable surface fraction is covered with liquid gallium, the As/Ga fluxes ratio on the (111)A surface exceeds this ratio on the (111)B surface.

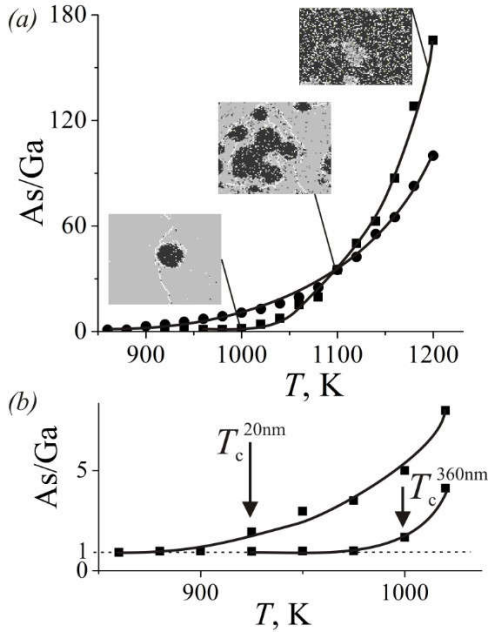

Fig. 2 *The temperature dependences of evaporated As/Ga ratio of two surface orientations ((111)A – squares, (111)B – circles) for L = 360 nm (a), and different terrace width for the (111)A surface (b). Top views of the model surface in (a) correspond to $T < T$*, $T = T$* and $T > T$*.*

4. Conclusions

The dependence of the main GaAs Langmuir evaporation characteristics on the substrate surface orientation was examined by Monte Carlo simulation. Ga droplets are easier created on the (111)B surface than on (111)A: congruent evaporation temperature T_c is lower and the droplet concentration higher. For the (111)A substrate orientation, the drop-crystal interface is rougher than that for (111)B. The congruent evaporation temperature was demonstrated to be the function of vicinal surface terrace width L. Dependence $T_c(L)$ is less pronounced for the (111)B surface. The high point defects concentration on the (111)A surface decreases value T_c. The change in the slope of As_2 evaporation rate temperature dependence for the (111)A surface orientation is revealed. This slope variation takes place at temperatures when an appreciable part of GaAs surface is covered with liquid gallium. Liquid gallium acts as a pump increasing arsenic evaporation from the (111)A surface. The features associated with the surface orientation can be explained by different Ga and As_2 volatilities and different rates of (111)A and (111)B surfaces etching by liquid gallium.

Acknowledgements

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