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Gallium desorption behavior at AlGaAs/GaAs heterointerfaces during high-temperature molecular beam epitaxy

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A Monte Carlo simulation study is performed to investigate the Ga desorption behavior during AlGaAs-on-GaAs heterointerface formation by molecular beam epitaxy. The transients in the Ga desorption rate upon opening the Al shutter are shown to be associated with the concurrent reduction in the V/III flux ratio. Monte Carlo simulations employing a constant V/III flux ratio yield a “steplike” variation in the Ga desorption rate with the resulting interfaces closer in abruptness to the ideal AlGaAs-on-GaAs interface. Further details on the stoichiometry of the interface and its relationship with predicted Ga desorption profiles is presented. © 1997 American Vacuum Society. [S0734-211X(97)09704-7]

I. INTRODUCTION

AlGaAs/GaAs heterostructures grown by molecular beam epitaxy (MBE) are important materials for applications in optical and electronic devices. It has been established for this system that growth at a high substrate temperature has important advantages. In addition to producing interfaces of high structural quality, employing high substrate temperatures also improves the optoelectronic properties of AlGaAs.^{1,2} An important problem that arises, however, is that these substrate temperatures are high enough to cause significant Ga desorption.^{3–7} Furthermore, *in situ* desorption mass spectrometry studies^{8,9} reveal that during AlGaAs-on-GaAs heterointerface formation the Ga desorption behavior is more complex than a simple constant or “steplike” behavior. Upon opening the Al shutter, there is a sharp rise in the Ga desorption rate, followed by a gradual decrease to a steady state value less than that corresponding to GaAs growth. A potential consequence of this transient is a compositional grading that extends 2–4 monolayers (ML) into the AlGaAs layer.

In a recent study¹⁰ we developed a Monte Carlo (MC) model to investigate the possible mechanisms that could explain the observed Ga desorption behavior at the AlGaAs-on-GaAs interface as seen during desorption mass spectrometry (DMS) experiments. The various factors investigated include the Al–Ga surface exchange mechanism, the effects of change in V/III flux ratio accompanying the opening of the Al shutter, and the influence of Al–Ga interaction energy. It was observed that the model including the Al–Ga surface exchange mechanism agreed well with the experimental results. Interesting was the fact that it was also observed that the experimental results could be reproduced

even without the Al–Ga surface exchange mechanism when the Al–Ga interaction energy was set to be equal to the Ga–Ga interaction energy. An examination of the predicted time evolution of the surface stoichiometry revealed that the transients in the Ga desorption rate were associated with a sharp decrease in the As coverage due to a reduction in the V/III ratio accompanying the opening of the Al shutter (to be discussed further later). The sharp rise in the Ga desorption rate was explained in terms of an instantaneous increase in the surface population of weakly bound Ga species due to the reduction in As coverage. The subsequent gradual decrease in the Ga desorption ratio was explained by the reduction in the number of surface cation sites from which Ga could desorb due to the presence of Al.

The above results indicate that the key to eliminating the Ga desorption transients at the AlGaAs-on-GaAs heterointerface is to maintain a constant V/III flux ratio. In this study we extend previously developed MC models¹⁰ to investigate different strategies that employ a constant V/III flux ratio. The effectiveness of the different strategies is examined by comparing the predicted Al/Ga concentration profiles at the AlGaAs-on-GaAs interface.

II. MODEL

The MC simulation procedure employed in the present study is similar to that adopted in previous models,^{11,12} wherein MBE growth is simulated by including deposition, surface migration, and desorption as allowed events. The model simulates growth on an unreconstructed (100) zinc-blende surface, explicitly taking into account the tetrahedral nature of the lattice with its individual sublattices for the cations and anions. An important difference between the present and previous models is that in the present model a temperature-dependent physisorption mechanism for cations

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is included to accurately model their desorption kinetics at high growth temperatures. In this mechanism a cation arriving at a cation terminated site is allowed a fixed number (temperature dependent) of jumps, determined by fit to experimental data, to find an anion terminated site; the cation desorbs if it is unsuccessful. The significance of this mechanism is that it accounts for the finite surface residence time for cations at high temperatures. By including this mechanism it was possible to obtain quantitative agreement with experimental Ga desorption rates for a range of growth temperatures,⁸ and also to accurately predict the dependence of Ga desorption energy on V/III flux ratio (for GaAs homoepitaxy) observed in experiments.⁵

Growth simulations were performed on a substrate 40×40 in size (site²) assuming a solid-on-solid (SOS) model (vacancies and overhangs not permitted) with periodic boundary conditions. The kinetic rates for deposition of Al, Ga, and As were assumed to be equal to their respective fluxes. The rates for surface migration and desorption events were assumed to be of the Arrhenius form with configuration-dependent activation energies calculated in terms of the first- and second-nearest-neighbor interaction energies, as in earlier MC models.^{11,12} The frequency factors and interaction energies for GaAs were taken from a previous study,¹⁰ and those for AlAs were determined from values for the cohesive energy.¹³ The model parameters used were the frequency factors for diffusion and desorption, $R_{\text{diff}} = 10^{10}/\text{s}$, $R_{\text{des}} = 7.5 \times 10^{12}/\text{s}$, respectively; nearest-neighbor interaction energies, $E_{\text{Ga-As}} = 0.85$ eV, $E_{\text{Al-As}} = 0.97$ eV; and second-nearest-neighbor interaction energies $E_{\text{Ga-Ga}} = 0.17$ eV, $E_{\text{As-As}} = 0.12$ eV, and $E_{\text{Al-Al}} = 0.25$ eV.

Our previous MC simulation study¹⁰ has shown that the Ga desorption behavior at the AlGaAs-on-GaAs interface is best described by two models (hereafter referred to as models I and II), where model I includes the Al–Ga surface exchange mechanism with the Al–Ga interaction energy ($E_{\text{Al-Ga}} = 0.21$ eV) set to be greater than the Ga–Ga interaction energy ($E_{\text{Ga-Ga}} = 0.17$ eV), and model II does not include the surface exchange mechanism with $E_{\text{Al-Ga}} = E_{\text{Ga-Ga}} = 0.17$ eV. In the present study we use both models to perform growth simulations in which the V/III flux ratio is held constant. MC simulations were performed employing two different procedures (hereafter referred to as cases 1 and 2); in case 1 the opening of the Al shutter is accompanied by an instantaneous increase in the As flux to maintain a constant V/III flux ratio, and in case 2 the As flux is maintained constant and the Al and Ga fluxes are adjusted such that the V/III ratio remains constant at a given x_{Al} .

In order to match the conditions used in a recent experiment,¹⁰ MC simulations were performed for growth temperatures in the range of 950–990 K at a V/III flux ratio of 5. Growth simulations at a given temperature were initiated by first growing several layers of GaAs (on a As terminated GaAs surface) with incident Ga flux at 1 ML/s. The final configuration of the GaAs surface was stored and was subsequently used as the starting surface in the AlGaAs growth simulations. During the initial stages of GaAs

growth, the Ga desorption rate increased sharply and reached a steady state value when the Ga incorporation into the substrate was about 1 ML. For convenience, time zero was defined to be the instant at which the Ga desorption ratio attained steady state value for that growth temperature.

The AlGaAs growth simulations for the two cases described above were performed under the following conditions. In case 1 the incident flux for Ga was 1.0 ML/s and that for Al 0.667 ML/s; in case 2 the incident flux for Ga was 0.6 ML/s and that for Al 0.4 ML/s. Both cases yield a nominal composition of $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$. In each simulation the Ga desorption ratio, defined as the fraction of incident Ga flux that desorbs, and the surface Al, Ga, and As fractions, defined as the fraction of surface sites terminated by the respective atomic species, were monitored as a function of time. The deposition of Ga was governed by the physisorption rule, while Al, which has a negligible desorption rate under the conditions of this study, was allowed enough jumps to find an appropriate SOS site. The Al–Ga surface exchange was implemented by having Al atoms that arrive at Ga terminated sites (by deposition or diffusion) replace the Ga atom. The ejected Ga atom then finds another site or desorbs, as per the physisorption rule.

III. RESULTS AND DISCUSSION

For completeness, we begin with a brief examination of results from growth simulations in which V/III flux ratio is not held constant. Figure 1(a) shows the time evolution of the Ga desorption ratio as predicted by models I and II. The experimental data are included for comparison. It is clear that a good match with experiment is obtained from both models. The origin of the transient in the Ga desorption ratio can be understood by examining the variation of the surface Al, Ga, and As concentrations with time, as shown in Fig. 1(b). The results from both models show that opening the Al shutter introduces an abrupt decrease in the As coverage due to a reduction in the V/III flux ratio. The observed transients can then be explained in terms of an abrupt increase in surface population of weakly bound Ga species followed by a decrease in the number of surface Ga sites, as described earlier.

Figure 2 shows the results from models I and II with the V/III flux ratios maintained constant using the two strategies specified in Sec. II. It is clear that both strategies eliminate the upward spike in the Ga desorption rate and result in a more rapid drop to the steady state value. However, both models predict that case 1 yields a steeper decline and a more steplike response in the Ga desorption behavior. The observed differences may be explained by examining the time evolution of the surface stoichiometry during growth. Figure 3 is a plot of the Al, Ga, and As concentrations of the surface versus time as predicted by model II. A comparison of the As coverage with that in Fig. 1(b) shows that both strategies are quite effective in eliminating drastic changes in the As coverage when the Al shutter is opened. Figure 3 also reveals that in case 2 the Ga surface concentration decreases more slowly and is also at a higher value than in case 1 before both profiles converge to the same steady state value.

FIG. 1. Models result from the simulation with the V/III flux ratio not held constant showing the time evolution of the (a) Ga desorption ratio and (b) surface stoichiometry. Experimental data in (a) are from Ref. 10. The horizontal lines in (b) were included for ease in delineating profiles corresponding to Al, Ga, and As.

The predicted Ga surface concentration profiles are thus consistent with the Ga desorption profiles shown in Figs. 2(a) and 2(b). The slower decrease in the Ga surface concentration for case 2 may be explained as follows. Given that the V/III flux ratio is the same for both cases, and that the group-III flux during AlGaAs growth is higher for case 1 (1.667 ML/s vs 1.0 ML/s for case 2), it follows that the amount of excess As, which is simply the As flux minus the group-III flux, is higher for case 1. This greater excess of As causes an increased incorporation rate for surface Ga, resulting in the effect observed.

In order to examine the effectiveness of the two strategies employed, it would be useful to compare the stoichiometry of the AlGaAs-on-GaAs interface predicted by the different models. The Al concentration profiles predicted by models I and II are shown in Figs. 4(a) and 4(b), respectively. For the case in which the V/III ratio is not held constant, we observe significant buildup of the Al concentration on the GaAs surface. In model II this buildup is confined mostly to the top GaAs layer, and is caused by Al atoms occupying cation sites left vacant by desorbing Ga atoms. The buildup in Al concentration is even more pronounced in model I due to the

FIG. 2. Model results for the two growth strategies that maintain a constant V/III flux ratio, as predicted by (a) model I (includes Al-Ga surface exchange) and (b) model II (excludes Al-Ga exchange).

presence of the Al-Ga exchange mechanism. Both models predict that maintaining a constant V/III flux ratio results in an interface that is closer to the ideal AlGaAs-on-GaAs interface. The best results are achieved in case 1, however,

FIG. 3. Evolution of the surface stoichiometry as predicted by model II (excludes Al-Ga surface exchange) with the V/III flux ratio maintained constant by two different methods. The horizontal lines were included for ease in delineating profiles corresponding to Al, Ga, and As.

FIG. 4. Al concentration profiles for conditions with and without the V/III flux ratio maintained constant, as predicted by (a) model I (includes Al-Ga exchange) and (b) model II (excludes Al-Ga exchange). The zero of the abscissa denotes the initial GaAs surface layer over which AlGaAs growth is simulated. The vertical line denotes the ideal AlGaAs-on-GaAs interface.

indicating that increasing the As flux is more efficient at suppressing both the Al-Ga exchange mechanism and Ga desorption from the GaAs surface. The influence of the As flux on the Al-Ga exchange mechanism as predicted by model I is in agreement with experimental studies^{14,15} that report a similar effect of the As overpressure on the exchange mechanism.

It is worth noting that there is a good correlation between the Al concentration profiles shown in Fig. 4 and their respective Ga desorption profiles presented in Figs. 1(a) and 2. The steeper decline in the Ga desorption ratio leads to a more abrupt interface. It should be noted, however, that a sharp rise in the Ga desorption rate (for conditions in which the V/III flux ratio is not held constant) does not lead to an overenrichment of Al at the interface as was predicted in a previous model.⁹ The previous model does not take into con-

sideration the penetration of impinging Al atoms into the GaAs surface and thus overestimates the Al enrichment at the AlGaAs-on-GaAs interface. Our models suggest that the spike in the Ga desorption profile leads to the formation of a diffuse interface of the order of 2–3 ML. It should be pointed out that the predictions of different models can be verified by performing appropriate growth experiments. While *in situ* DMS can be used to verify the predicted Ga desorption profiles, the stoichiometric profiles can be verified by high-resolution transmission electron microscopy using the chemical lattice imaging technique.¹⁶

IV. SUMMARY

The transient in the Ga desorption rate during AlGaAs-on-GaAs heterointerface formation is caused by a reduction in the V/III flux ratio that coincides with the opening of the Al shutter. The present MC study shows that “steplike” variations in the Ga desorption rate and abrupt interfaces can be realized by adopting conditions in which the V/III ratio is maintained constant during growth. The best results are obtained when the reduction in the V/III ratio is compensated by an increase in the As flux.

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