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Low-temperature molecular beam epitaxy of GaAs: A theoretical investigation of antisite incorporation and reflection high-energy diffraction oscillations

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Surface dynamics dominate the incorporation of charged, As_{Ga}^+ , and neutral, As_{Ga}^0 , antisite arsenic, and the temporal variation of reflection high-energy electron diffraction (RHEED) intensity in the low-temperature molecular beam epitaxy of (100) gallium arsenide (GaAs). A rate equation model is proposed which includes the presence and dynamics of a physisorbed arsenic (PA) layer riding the growth surface. The PA layer dictates the incorporation and concentration of As_{Ga}^+ and As_{Ga}^0 . Additionally, it influences the RHEED oscillations (ROs) behavior and the RO's dependence on its coverage through its contribution to the reflected intensity. The model results for the dependence of As_{Ga}^+ and As_{Ga}^0 concentrations on beam equivalent pressure (BEP) and growth temperature are in good agreement with experimental data. The experimental observations can be explained based on the saturation of the PA coverage at one monolayer and the competing rate processes such as the As_{Ga} incorporation into and evaporation from the crystalline surface. Using the same kinetic model for the temporal behavior of the surface, the contribution of the PA layer to the RHEED intensity is computed based on kinematical theory of electron diffraction. The experimental observation of the ROs during growth at high and low temperatures with no ROs in the intermediate temperature range of 300–450 °C is in good agreement with our model results. At low temperatures, the surface is covered by the PA layer whose step density depends on that of the subsurface crystalline GaAs. Thus, a temporal variation of the step density of subsurface crystalline GaAs results in ROs, but with a different step height, that of the PA layer, of 2.48 Å. At high temperatures, the crystalline GaAs is exposed to the RHEED beam due to the evaporation of the PA layer and the ROs appear due to periodic step-density oscillations with a step height of 1.41 Å, which is the Ga–As crystalline interplanar distance. At intermediate temperatures, the surface is partially covered by the PA layer resulting in RHEED reflection contributions from both surfaces covered by the PA layer and crystal. Due to the very different interplanar distances between the crystalline GaAs and the PA layers, complete destructive interference of the RHEED intensity results at a 0.5 surface coverage of the PA layer. The RO dependence on the As BEP is also presented and discussed. © 1999 American Vacuum Society. [S0734-211X(99)04103-7]

I. INTRODUCTION

In 1978, Murotani, Shimanoe, and Mitsui¹ observed the semi-insulating properties of nonstoichiometric low-temperature-grown GaAs (LT-GaAs) in the temperature range of 400–600 °C. The LT-GaAs grown at about 200 °C was found to have buffer-layer applications in metal–semiconductor field-effect transistors (MESFETs),² to eliminate the problem of sidegating, and in high electron mobility transistors (HEMTs).³ These beneficial properties are directly related to the excess arsenic incorporated during LT-GaAs molecular beam epitaxy (MBE) growth. The excess As precipitates when annealed at 400–600 °C.⁴ The excess As results in point defects⁵ in the form of antisite arsenic As_{Ga} , arsenic interstitials As_i , and gallium vacancies V_{Ga} .^{6,7} As_{Ga}

have been accepted as the dominant defects⁸ in these materials. Since gallium vacancies are triple acceptors, a part of As_{Ga} is charged as As_{Ga}^+ (Ref. 9) to maintain the charge neutrality of the material. The ultrafast trapping characteristics of carriers in these materials, which are useful for applications, have been correlated to the presence of As_{Ga}^+ .⁹ It is shown that doping the material suitably with Be increases the As_{Ga}^+ concentration,¹⁰ and hence, decreases the carrier lifetime. Muthuvenkatraman *et al.*¹¹ simulated the growth of LT-GaAs using a stochastic model and explained the growth condition dependence of the antisite concentrations based on the presence of a physisorbed As layer and its surface dynamics.

Ibbetson *et al.*¹² observed that during MBE growth using near-stoichiometric flux ratio conditions, reflection high-energy electron diffraction (RHEED) oscillations (RO) can be observed at temperatures as low as 200 °C. Pamula, Ven-

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katasubramanian, and Dorsey¹³ used a stochastic model of growth allowing for a physisorbed As (PA) layer. It was shown that the ROs were enhanced by the temporal oscillations of the PA layer coverage, which exposed oscillating crystalline surface coverage exposed to the RHEED beam. Recently, Shen *et al.*¹⁴ have shown that the stoichiometric flux condition is not a prerequisite for the RO observation and that the ROs can be observed over a wide range of beam equivalent pressures (BEP) and temperatures. They also observed that the ROs are suppressed over a temperature window at a fixed BEP and over a BEP window at a fixed temperature.¹⁴ The aim of this article is to modify the theoretical rate equation model of Ref. 13 to make it a comprehensive model which will capture not only the physics of antisite incorporation, but also the RO behavior. The formulation of the model and the details are presented in Sec. II. Results and discussion are presented in Sec. III. Finally, conclusions are presented in Sec. IV.

II. RATE EQUATION MODEL FOR GROWTH OF GaAs

The rate equation model used to study the LT-GaAs growth by MBE considers surface kinetic processes: adsorption, evaporation, and interlayer and intralayer surface migration. The model considers, in addition to the kinetics of

the above processes, the presence and kinetics of a physisorbed layer of As consisting of weakly bound atoms by van der Waal-type binding. The time evolution of the epilayer is described through the change of macrovariables caused by the surface processes. The macrovariables of growth are normalized with respect to the maximum number of possible atoms in the layer. The macrovariables considered are the layer coverage of atoms in Ga, As, and As_{Ga} layers given as

$C_{\text{Ga}}(2n)$: layer coverage of Ga in the $2n$ th layer,

$C_{\text{As}}(2n)$: layer coverage of As in the $2n+1$ th layer,

$C_{\text{AsGa}}(2n)$: layer coverage of antisite in the $2n$ th layer, (1)

where n is the layer index, with the regular Ga and antisite As belonging to even layers, and the regular As belonging to the odd layers. The layer coverage of atoms is 1, when the layer is completely full and 0, when the layer is completely empty. The adsorption rate depends on the flux rate and the number of sites available at the surface for proper covalent bonds. The rates of evaporation and migration are considered to be Arrhenius with frequency factors and activation energies. The time evolution of the layer coverage of Ga in the $2n$ th layer due to the various surface processes is given by

$$\begin{aligned} \frac{dC_{\text{Ga}}(2n)}{dt} = & \{ [C_{\text{As}}(2n-1) - C(2n)] J_{\text{Ga}} \} (A) + [C_{\text{As}}(2n-1) - C(2n)] \left\{ R_0 e^{-E_d(2n+2)/kT} \left(\frac{C_{\text{Ga}}(2n+2)}{C(2n+2)} \right) [C(2n+2) \right. \\ & - C_{\text{As}}(2n+3)] + R_0 e^{-E_d(2n-2)/kT} \left(\frac{C_{\text{Ga}}(2n-2)}{C(2n-2)} \right) [C(2n-2) - C_{\text{As}}(2n-1)] \right\} (B) - R_0 e^{-E_d(2n)/kT} \left(\frac{C_{\text{Ga}}(2n)}{C(2n)} \right) \\ & \times [C(2n) - C_{\text{As}}(2n+1)] \{ [C_{\text{As}}(2n+1) - C(2n+2)] + [C_{\text{As}}(2n-1) - C(2n)] \} (C) \\ & - R_0 e^{-E_e(2n)/kT} \left(\frac{C_{\text{Ga}}(2n)}{C(2n)} \right) [C(2n) - C_{\text{As}}(2n+1)] (D). \end{aligned} \quad (2)$$

The terms A , B , C , and D represent the change of Ga coverage due to incorporation of As, migration into and out of the $2n$ th layer, and evaporation from the exposed layer, respectively, and R_0 is the frequency factor. E_d and E_e are the activation energies for diffusion and evaporation, respectively, and given by

$$E_d(2n) = E_{d,\text{iso}} + 4E_{\text{GaGa}}C_{\text{Ga}}(2n),$$

$$E_e(2n) = E_{e,\text{iso}} + 4E_{\text{GaGa}}C_{\text{Ga}}(2n),$$

and thus, making the energies a function of the layer coverages: the activation energies of the isolated atoms $E_{d,\text{iso}}$ and the second-neighbor atom-atom pair interaction energy. Two more time evolution equations similar to Eq. (1) are written for the other macrovariables, viz., the layer coverages of arsenic in the $2n+1$ th layer, $C_{\text{As}}(2n+1)$ and antisite arsenic in the $2n$ th layer, $C_{\text{AsGa}}(2n)$. An additional equation

describes the growth kinetics of a physisorbed arsenic layer, which includes the weakly bound physisorbed state for As₂ from which arsenic can either chemisorb onto the crystal or evaporate.¹⁷

III. COMPUTATIONS, RESULTS, AND DISCUSSIONS

In this work, the growth direction is chosen as $[100]$. A total of 241 ($=80 \times 3 + 1$) differential equations describing the time evolution of the macrovariables corresponding to 80 GaAs bilayers and the PA layer are used for the simulation of the growth. These equations are coupled nonlinear first-order differential equations. By solving these equations numerically using a fourth-order Runge-Kutta method, the time evolution of the macrovariables is obtained, which in turn can be used to obtain the time evolution of the surface coverage. The average concentrations of Ga, As, and As_{Ga} in individual layers at the end of growth are obtained from the

solution of the differential equations by considering the layers in the bulk, viz., the layers far from the substrate and the surface. From these results, the neutral and charged antisite concentrations and the intensity of RHEED versus time results can be computed for various growth conditions.

A. Neutral and charged antisite concentrations

The growth rate is chosen to be 1 $\mu\text{m/h}$. As is assumed to be a monomer, cracked from either As_2 or As_4 . Both Ga and As are allowed to incorporate on the surface sites even when only one of the surface covalent bonds is satisfied. Investigations are performed over a temperature ranging from 423 to 513 K for the calculations of antisite concentrations over a BEP ranging from 9 to 30.

From the solutions of the differential equations, the coverage of Ga, As, and As_{Ga} in their respective layers for all 80 bilayers are obtained as a function of time using the procedure explained in Sec. III. In the case of even numbered layers, i.e., Ga sublattices, in addition to Ga and As_{Ga} , there are vacancies V_{Ga} present. Hence, the coverage of the even numbered layers $C(2n)$ is given by

$$C(2n) = C_{\text{Ga}}(2n) + C_{\text{As}_{\text{Ga}}}(2n). \quad (3)$$

The coverage of V_{Ga} in the $2n$ th layer is the sum of all Ga sites not occupied by either Ga or As_{Ga} and is, therefore, given by

$$C_{V_{\text{Ga}}} = 1 - C(2n), \quad (4)$$

since the maximum coverage possible in a layer is 1. The Ga vacancies V_{Ga} present in the bulk are triple acceptors,⁹ and hence, partially compensate As_{Ga} , resulting in As_{Ga}^+ . In other words, from the charge neutrality equation, the charged antisite As_{Ga}^+ coverage should be equal to three times that of V_{Ga} , which is written mathematically as

$$3C_{V_{\text{Ga}}}^{3-} = C_{\text{As}_{\text{Ga}}}^+. \quad (5)$$

$C_{V_{\text{Ga}}}^{3-}$, and hence, $C_{\text{As}_{\text{Ga}}}^+$ can be obtained from the simulation results using Eqs. (3)–(5). The total antisite coverage in the $2n$ th layer, which is obtained as part of the results of simulation, is the sum of charged and neutral antisites:

$$C_{\text{As}_{\text{Ga}}}(2n) = C_{\text{As}_{\text{Ga}}}^+(2n) + C_{\text{As}_{\text{Ga}}}^0(2n). \quad (6)$$

Hence, the coverage of neutral antisites $C_{\text{As}_{\text{Ga}}}^0$ can be obtained using Eqs. (5) and (6). The layer coverages of antisites for several layers far away from the surface and substrate, i.e., bulk, were found to be uniform for all simulations. These coverages of the bulk layers were averaged and converted to volume concentrations.

Charged and neutral antisite As concentration versus BEP obtained from our simulations were fitted to four experimental data points of Luysberg *et al.*¹⁵ to fix the model parameters accurately. The values for the model parameters are listed in Table I. Using these parameters, model predictions for the remaining growth conditions were obtained.

Simulation results for the As_{Ga}^+ concentration as a function of BEP and versus temperature are shown in Fig. 1. Similar

TABLE I. Model parameters obtained by fitting the simulation results to the experimental data of Luysberg *et al.* (Ref. 9) and Specht *et al.* (Ref. 10).

Parameter	Description	Model value
$\tau_{o,\text{in}}^{\text{As}_{\text{Ga}}}$	Prefactor for antisite adsorption	172.0 s
$\tau_{o,\text{ev}}^{\text{phy,As}}$	Prefactor for physisorbed As evaporation	2.1×10^{-4}
$\tau_{o,\text{in,reg}}^{\text{phy,As}}$	Prefactor for physisorbed As incorporation in regular As site	172.0 s
$E_{d,\text{iso}}^{\text{Ga}}$	Activation energy for diffusion for isolated Ga atom	0.4 eV
$E_{d,\text{iso}}^{\text{As}_{\text{Ga}}}$	Activation energy diffusion for isolated As_{Ga} atom	1.45 eV
$E_{d,\text{iso}}^{\text{As}}$	Activation energy for diffusion for isolated As atom	0.8 eV
$E_{e,\text{iso}}^{\text{Ga}}$	Activation energy for evaporation for isolated Ga atom	1.4 eV
$E_{e,\text{iso}}^{\text{As}_{\text{Ga}}}$	Activation energy diffusion for isolated As_{Ga} atom	1.3 eV
$E_{e,\text{iso}}^{\text{As}}$	Activation energy for diffusion for isolated As atom	1.5 eV
$E_{\text{Ga-Ga}}$	2nd-neighbor atom–atom pair interaction energy for Ga	0.14 eV
$E_{\text{As-As}}$	2nd-neighbor atom–atom pair interaction energy for As	0.25 eV
$E_{\text{As-As}_{\text{Ga}}}$	2nd-neighbor atom–atom pair interaction energy for As and As_{Ga}	0.25 eV
$R_0^{d,\text{Ga}}$	Frequency factor for Ga for diffusion	2537.0/s
$R_0^{e,\text{Ga}}$	Frequency factor for Ga for evaporation	463970.0/s
$R_0^{d,\text{As}_{\text{Ga}}}$	Frequency factor for As_{Ga} for diffusion	7.8×10^{14} /s
$R_0^{e,\text{As}_{\text{Ga}}}$	Frequency factor for As_{Ga} for evaporation	1.1×10^{12} /s
R_0^{As}	Frequency factor for As	4.16×10^{10} /s

behavior was observed for the As_{Ga}^0 concentration. Both As_{Ga}^0 and As_{Ga}^+ concentrations saturate beyond a BEP of 20 for all temperatures. The explanation for such a behavior can be given based on the consideration of the PA layer of arsenic. For a given temperature, as BEP increases, the As flux in excess of Ga flux increases, resulting in an increase in the PA layer coverage until the coverage reaches its maximum value of unity at a critical BEP. Beyond the critical BEP, any further increase in BEP does not change the PA layer coverage as it has attained its maximum. The As_{Ga}^0 and As_{Ga}^+ concentrations incorporated in the crystal are dictated by two competing mechanisms, incorporation of As from the PA layer and evaporation of As_{Ga} from the crystal. For a given temperature, the saturation of As_{Ga} occurs because the incorporation and evaporation lifetimes and the PA layer coverage are all constant beyond the critical BEP. Hence, the incorporation of As_{Ga}^0 and As_{Ga}^+ directly depends on the PA layer coverage. The saturation of As_{Ga} concentration is lower for

FIG. 1. Model results for charged antisite concentration as a function of BEP and temperature.

higher temperature because of the higher evaporation rate of As_{Ga} from the crystal. The decrease in As_{Ga}^+ concentration with increase in temperature is also due to the larger migration length for Ga at higher temperatures, which decreases the Ga vacancy concentration, and hence, decreases the As_{Ga}^+ concentration. Both As_{Ga}^+ and As_{Ga}^0 exhibit the same dependencies on BEP and temperature, but the As_{Ga}^0 concentration is consistently one order of magnitude higher than the concentration of As_{Ga}^+ .

When the temperature decreases from 513 K, the concentrations of both As_{Ga}^0 and As_{Ga}^+ continue to increase until a particular value and then saturate at all BEP values. This result is in agreement with the experimental results.¹⁵ As the temperature decreases from 513 K, the evaporation of As_{Ga}^0 from the crystal decreases and becomes negligible at lower temperatures, and hence, the As_{Ga}^0 concentration increases. At low temperatures, the PA layer coverage is more and at a critical temperature, it reaches the monolayer coverage, which makes the antisite concentration saturate.

A plot of the concentration of As_{Ga}^0 versus BEP for various growth rates in the range of 1–1.5 $\mu\text{m}/\text{h}$ is shown in Fig. 2. The As_{Ga}^0 concentration decreases when the growth rate is increased at all the values of BEP uniformly. When the growth rate is increased, say from 1 $\mu\text{m}/\text{h}$, the number of Ga atoms arriving at the surface increases. There is a competition between the arriving Ga atoms and the antisite As to occupy the surface cationic sites of the growing crystal. When more numbers of Ga atoms arrive at the surface, the incorporation of excess As into antisites decreases, and hence, the As_{Ga}^0 concentration decreases. The growth rate dependence of As_{Ga}^+ concentration was observed to be similar to that of the As_{Ga} and the physical explanation is also similar.

B. RHEED oscillations

The kinetics of the PA layer are critical to the overall growth kinetics. The presence of the PA layer on the surface

FIG. 2. Model results for neutral antisite concentration as a function of BEP at different growth rates.

influences the RHEED response. The incident RHEED electron beam interacts with both the crystalline surface of the growing crystal and the surface of the PA layer. Hence, the amplitude of ROs is dictated not only by the step density variation, but also by the physisorbed layer coverage with time. The crystalline surface of the GaAs exposed to the RHEED beam changes with time due to the periodic variation of the surface coverage of the PA layer. A schematic picture of the RHEED beam interactions with the two surfaces is illustrated in Fig. 3. The growth rate considered for this study is 0.7 $\mu\text{m}/\text{h}$, the same as that used in the experimental work of Shen *et al.*¹⁴ The primary electron energy of the monoenergetic electron beam directed towards the surface is taken to be 10 kV at a grazing incidence angle of 1° .

The intensity of the RHEED specular beam can be calculated using the kinematic theory of electron diffraction written from the two distinct surfaces, the PA surface, and the exposed crystalline surface, as

$$A_1(t) = \sum_{n=1}^{n=\infty} [C(2n-1) - C(2n)](1 - C_{\text{phy}}) \times \exp\left[i\left((2n-1)\frac{2\pi}{\lambda}d\right)\right], \quad (7)$$

FIG. 3. Schematic picture showing the reflected electron beams from the PA layer and from the crystalline surface and the thicknesses of the layers.

FIG. 4. ROs at 40 BEP for various temperatures at a growth rate of 0.7 $\mu\text{m/h}$, compared qualitatively with the experimental results of Fig. 3 of Shen *et al.* (Ref. 14).

$$A_2(t) = \sum_{n=1}^{n=\infty} [C(2n-1) - C(2n)](C_{\text{phy}}) \times \exp \left[i \left((2n-1) \frac{2\pi}{\lambda} d + d_{\text{phy}} \right) \right], \quad (8)$$

where the term A_1 accounts for the scattered wave amplitude from the exposed crystal and A_2 for that from the PA layer. C_{phy} is the surface coverage of the PA layer. d_{phy} is the interplanar distance of the PA layer and the underlying crystalline layer. d is the interplanar distance of the GaAs crystal. λ is the wavelength of the incident beam in radians. Then, the resultant specular beam intensity I is given by

$$I(t) = \sum_{n=1}^{n=\infty} |A_1(2n) + A_2(2n)|^2. \quad (9)$$

Note that the coverage variables are a function of time, and hence, $A_1(t)$, $A_2(t)$, and $I(t)$ will also be functions of time.

The time evolution of the RHEED intensity can be computed based on the kinematical theory of diffraction with an As–As interplanar distance of 2.48 Å for the physisorbed As layer and a Ga–As interplanar distance of 1.41 Å. The interplanar distances considered are quite reasonable since in the PA layer atoms are loosely connected with van der Waal-type binding, and hence, the value should be larger than the crystalline Ga–As bond and close to the gaseous dimer As_2 bond length.

Plots of ROs versus time at a BEP of 40 with varying temperatures simulated using our model are shown in Fig. 4. Comparing the results of Fig. 1 of Ref. 14 to Fig. 4, the qualitative agreement between the results is good. At an As BEP of 40, the ROs are prominent for temperatures above 773 K and below 573 K with a temperature window between 573 and 723 K in which ROs disappear. This behavior can be explained as follows. The growing GaAs surface is par-

tially covered by a layer of physisorbed As which is bonded to chemisorbed crystalline As. Thus, the reflected RHEED intensity has two components, one from the exposed GaAs crystalline surface and the other from physisorbed As. For low temperatures, the surface is almost covered by the physisorbed As whose step density oscillates periodically with the subsurface crystalline GaAs, and hence, results in ROs. At high temperatures, the physisorbed As evaporates from the surface and exposes the crystalline GaAs, which yields ROs due to periodic step-density oscillations. At intermediate temperatures, the surface is partially covered by the physisorbed As layer resulting in RHEED intensity components from both the crystalline and physisorbed As surfaces. Due to the very different interplanar distances between these layers, i.e., $d_{\text{Ga-As}} = 1.41 \text{ Å}$ and $d_{\text{As-As}} = 2.48 \text{ Å}$, complete destructive interference of the two reflected components of the beam results at a PA surface coverage of 0.4 layers. Thus, there are no ROs in the intermediate temperature range of 573–773 K.

A few comments on the model employed for the study are in order here. The proposed model is based on several experimental observations^{12,16–19} and physically sound. It explains several independent experimental observations consistently.^{9,10,12,14} The model is simple and ignores the presence and influence of the surface reconstructions. It is believed that the most probable surface reconstruction for most of the growth conditions simulated by the model will be $c(4 \times 4)$ and its variants. Even though the model parameters can change from one variant to another, it is believed that these changes are expected to be small, and hence, are ignored to keep the model simple. Additionally, to keep the model simple for RHEED intensity calculations, multiple reflections are ignored. It was found that a small variation in the incident angle or the unknown, but well-estimated, interplanar distance for the physisorbed arsenic d_{phy} has minimal impact on the results. It is noted that variations in d_{phy} will change the temperature range in which the ROs are suppressed.

IV. CONCLUSIONS

A modified stochastic model based on surface processes is developed to explain the physics of the antisite incorporation and ROs behavior LT-GaAs MBE under various growth conditions. The PA layer of As weakly bound at the surface of the growing crystal and its surface dynamics strongly influence the incorporation of As_{Ga}^0 and As_{Ga}^+ and the resultant ROs. The observation of saturation of antisite concentration with BEP can be explained based on the surface coverage saturation of the PA layer and the evaporation of antisites from the crystalline layer. The PA layer has a larger value (2.48 Å) interplanar distance than the crystal (1.41 Å) because of the weakly bound atoms. Based on the kinematical theory of diffraction, this time evolving physisorbed layer of arsenic affects the RHEED intensities with constructive and destructive interference. At an intermediate temperature of about 573–723 K, ROs disappear due to destructive interference between the beam components reflected from the crys-

talline surface and from the PA layer. The model explains three sets of independent experimental observations, i.e., antisite concentrations versus growth conditions and RO's versus growth condition.^{9,12,14}

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