Passivation of surface defects on InGaAs (001) and (110) surfaces in preparation for subsequent gate oxide ALD

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INTRODUCTION

$In_{0.53}Ga_{0.47}As$ contains an intrinsically high electron mobility making it an attractive alternative semiconductor material for use in the channel region of MOSFET devices[1]. The semiconductor/oxide interface can degrade device performance through interfacial roughness or formation of surface defects containing electronic trap states that act to pin the surface Fermi level[2]. Tri-gate structured field effect transistors (finFETs) are currently being implemented into commercialized logic chips, making defect reduction and passivation of the semiconductor planar and sidewall crystallographic faces critical in order to create an ideal interface between the semiconductor and the gate oxide. For InGaAs(001) based finFETs to become potential for commercial implementation, in-situ III-V surface cleaning or defect passivation techniques must be compatible with both the InGaAs (001) and (110) surfaces. STM was employed to show air exposed InGaAs (001) and (110) samples can be restored to the cleanliness of MBE grown samples through atomic hydrogen dosing and thermal annealing. STM was also employed to characterize the in-situ self-limiting CVD of a silicon hydride control layer used to passivate the missing dimer defect unit cells of the arsenic rich InGaAs(001)-(2x4) surface. Surface defect densities are compared and quantified throughout several STM images following the surface cleaning and passivation techniques.

EXPERIMENTAL

This study employs n-type (silicon dopant) samples consisting of 0.2 μm of 1-$2x10^{18}$ doped $In_{0.53}Ga_{0.47}As$(001) layers, and 0.1 μm of $1x10^{18}$ doped $In_{0.53}Ga_{0.47}As$(110) layers grown by MBE on InP substrates. All samples were capped with an As_2 layer and shipped/stored under vacuum. In the preparation chamber, all samples were degassed and, subsequently, the (001) samples were decapped and annealed for one hour at 360-370°C to obtain the InGaAs(001)-(2x4) surface reconstruction. The (110) samples were decapped and annealed for one hour at 360-370°C to obtain the bare InGaAs(110) surface. Following decapping and annealing, samples were exposed to air for 30 minutes to form a surface oxide layer. An Oxford Applied Research TC-50 thermal gas cracker operated at 65 Watts was employed to produce atomic hydrogen from H_2 gas. The air exposed (001) and (110) samples were exposed to $1x10^{-6}$ torr H_2 for 10-30 minutes at various temperatures and STM was used to quantify surface defects. STM images were obtained in constant current mode with a current set point of 100 pA and sample bias of -3 V for filled state imaging. Two new in-situ surface defect passivation techniques for the decapped InGaAs(001)-(2x4) surface were employed by self-limiting CVD of a silicon hydride seed layer. Silicon hydride surface saturation was confirmed by XPS using the aluminum Kα excitation source (hv=1486.7 eV) with spectra taken at a glancing angle of 30° to obtain enhanced surface sensitivity. For the 250°C self-limiting CVD process, the decapped $In_{0.53}Ga_{0.47}As$(001)-(2x4) surface underwent a series of Si_3H_8 doses at 250°C and after the total saturated 300 MegaLangmuir Si_3H_8 dose, STM was performed to study the surface order and to quantify surface defects. For the 350°C self-limiting CVD process, the decapped $In_{0.53}Ga_{0.47}As$(001)-(2x4) surface underwent a series of Si_2Cl_6 doses at 350°C and after the total saturation 21 MegaLangmuir Si_2Cl_6 dose, 500 Langmuir atomic hydrogen was dosed at 350°C to remove chlorine termination by replacing with atomic hydrogen. After the atomic hydrogen dose, STM was performed to quantify surface defects present. The quantifications in Table 1 were obtained by manually counting the number of islands and dark sites in the corresponding 100 x 100 nm^2 STM images and extrapolating these numbers to 1 $μm^2$. The surface islands are defined as any group of atoms on a terrace greater than 3 nm^2 while the dark sites are surface vacancies ranging from 0.01-3 nm^2. The percentage of missing dimer unit cells was calculated from manually counting the number of missing dimer unit cells and dividing by the total number of unit cells in each STM image. Quantifications for decapped (001)/(110) surfaces, and air exposed (001)/(110) surfaces before and after atomic hydrogen dosing and annealing were reported previously and are shown here to provide a complete defect density comparison across all InGaAs surface passivation and cleaning techniques[3,4].

RESULTS AND DISCUSSION

Figure 1(a) shows a filled state STM image of the decapped InGaAs(001)-(2x4) surface. The surface arsenic dimer rows have a characteristic zig-zag shape due to a mixture of double As dimer and single As dimer defect unit cells. Figure 1(b) shows an enlarged inset taken from Figure 1(a) highlighting the ideal double dimer unit cell and the missing dimer defect unit cell found on the InGaAs(001)-(2x4) surface. The decapped surface contains roughly 70% of the defect missing dimer unit cells across the surface, as measured by manually counting the defect unit cells from the total number of unit cells found in the STM image[3]. DFT calculations show the missing dimer defect unit cells produce unwanted conduction band edge states which act to pin the surface Fermi level[3]. Figure 2(a) shows a filled-state STM image of the InGaAs(001)-(2x4) surface following a saturated 300 MegaLangmuir Si_3H_8 dose at 250°C. The surface contains 25% less incomplete terrace surface islands than the decapped surface, and a low density of surface dark sites. Similarly, Figure 2(b) shows a filled-state STM image of the InGaAs(001)-(2x4) surface following the 21 MegaLangmuir saturated Si_2Cl_6 dose and 500 Langmuir atomic hydrogen dose at 350°C. The surface contains high atomic order with roughly the same amount of incomplete surface terraces as the decapped surface, and a higher amount of surface dark sites probably due to surface etching from chlorine. Initial DFT calculations will be presented which show $Si-H_x$ groups passivate the missing dimer defect unit cell of the InGaAs(001)-(2x4) surface. Figure 3(a) shows the InGaAs(001)-(2x4) surface following 30 minute air exposure. The surface contains an amorphous oxide layer. Figure 3(b) shows the air exposed surface following a 30 minute 1800 Langmuir atomic hydrogen dose at 285°C. The surface contains a comparable amount of missing dimer unit cells to the clean decapped surface and about

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3.5x higher incomplete atomic terraces[3]. Figure 3(c) shows the hydrogen cleaned air exposed InGaAs(001)-(2x4) surface following a 30 minute post anneal at 290°C. This post anneal had no change on the number of defect unit cells but the incomplete atomic terraces were reduced by 25%[3]. Figure 4(a) shows the decapped InGaAs(110) surface and the two types of intrinsic defects on this surface are bright sites (circle) and dark sites (box) are highlighted. The dark site defects are several orders of magnitude greater than the bright site defects. The decapped InGaAs(110) surface becomes amorphous following 30 minute air exposure (not shown). Figure 4(b) shows the air exposed surface following a 600 Langmuir atomic hydrogen dose at 275°C with no further annealing. The surface was returned to order without need for a post cleaning anneal, and with small atomic terraces seen across the surface. The hydrogen cleaned (110) surface contains no dark site defects, and contains 25x more incomplete atomic terraces than the decapped (110) surface most likely due to lower diffusion rates on the InGaAs(110) surface. A subsequent anneal to 350 ˚C for 30 min was performed, but no significant change in defect densities was seen.

Conclusion

Hydrogen cleaning and post annealing has been demonstrated as an effective way to clean air exposed InGaAs (001) and (110) surfaces providing an in-situ cleaning method compatible with three dimensional device structures. For the air exposed InGaAs(001)-(2x4) surface, hydrogen cleaning and post annealing process significantly reduces the dark sites and incomplete terraces formed from the hydrogen cleaning procedure, although the percentage of defect unit cells remains high. For the air exposed InGaAs(110) surface, hydrogen cleaning effectively removes the surface oxide and eliminates the need for a post cleaning anneal. The high defect density after hydrogen cleaning compared to the decapped (110) surface is consistent with lower diffusion rates for substrate atoms on InGaAs (110) than InGaAs (001). Both self-limiting CVD processes on InGaAs(001)-(2x4) are shown to produce atomic surface order with low surface defect densities. The 250°C Si_3H_8 process only requires the use of a single ALD precursor, Si_3H_8, and self-limiting growth is achieved at a very low temperature. The 350°C process allows for multilayer silicon growth by ALD through cyclically dosing Si_2Cl_6 and atomic hydrogen, as shown by Koleske et al.[5]. Both self-limiting CVD processes result in the deposition of a thin atomically ordered silicon hydride seed layer on InGaAs(001)-(2x4). Initial DFT calculations will be presented and show the InGaAs(001)-(2x4) missing dimer unit cell is electronically passivated by $Si-H_x$ groups, making this passivation method promising for passivation of dangling bonds on the (110) surface and creating a passivating silicon control monolayer capable of seeding ALD nucleation.

References

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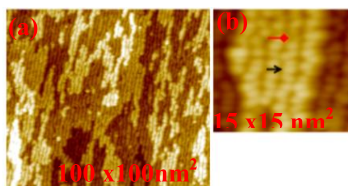

Figure 1 (a) STM image of decapped InGaAs(001)-(2x4). (b) Inset of (a) with black arrow pointing to an ideal double As dimer unit cell site and diamond head arrow pointing to a defect single As dimer unit cell site.

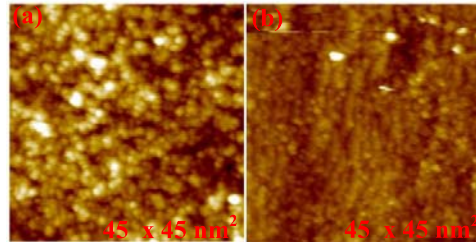

Figure 2 (a) STM of decapped InGaAs(001)-(2x4) following 300 MegaLangmuir Si_3H_8dose at 250°C. (b) STM of decapped InGaAs(001)-(2x4) surface following 21 MegaLangmuir Si_2Cl_6 and 500 Langmuir atomic hydrogen at 350°C.

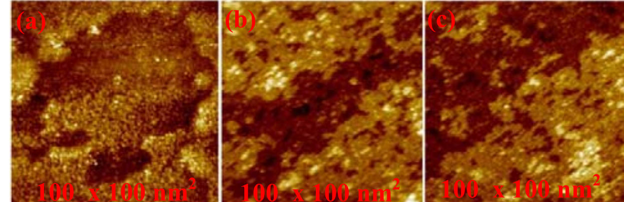

Figure 3 (a) STM image showing decapped InGaAs(001)-(2x4) surface following 30 minute air exposure. (b) STM image showing air exposed surface following 1800 Langmuir atomic hydrogen dose at 285°C. (c)STM image showing air exposed surface following 1800 Langmuir atomic hydrogen at 285°C, and 30 minute anneal at 290°C

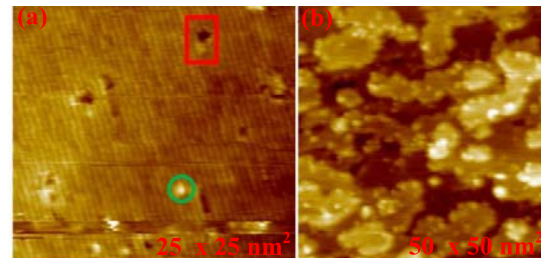

Figure 4 (a) STM image showing the decapped InGaAs(110) surface. (b) STM image showing air exposed surface following 600 Langmuir atomic hydrogen dose at 275°C.

Surface	Unit Cells	Missing Dimer Unit Cells	% Missing Dimer Unit Cells	Density of Dark Sites (/µm²)	Density of Incomplete Terraces (/µm²)
Decapped InGaAs(001)-(2x4)	872	619	71%+/-6%	0	1,700
285°C H Clean air exposed InGaAs(001)-(2x4)	806	645	80%+/-4%	12,400	6,000
285°C H Clean + Post Anneal air exposed InGaAs(001)-(2x4)	806	632	78%+/-5%	5,600	4,500
300 MegaLangmuir Si_3H_8 /InGaAs(001)-(2x4)	N/A	N/A	N/A	1,975	1,481
21 MegaLangmuir Si_2Cl_6 dose + 500 Langmuir H /InGaAs(001)-(2x4)	N/A	N/A	N/A	4,938	1,975
Decapped InGaAs(110)	N/A	N/A	N/A	11,613	200
600 Langmuir Atomic H dose at 285°C on air exposed InGaAs(110)	N/A	N/A	N/A	N/A	5,000

Table1 Quantification of surface defects as a function of surface preparation method