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Real Space Surface Reconstructions of Decapped As-rich $In_{0.53}Ga_{0.47}As(001)$-(2×4)

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The surface reconstructions of decapped $In_{0.53}Ga_{0.47}As(001)$ have been studied using scanning tunneling microscopy (STM). It is shown that the As-rich α2(2×4) and β2(2×4) reconstructions, predicted by density function theory (DFT) (1-3) for GaAs(001)-(2×4), InAs(001)-(2×4) and InGaAs(001)-(2×4) surfaces, were observed to coexist on $In_{0.53}Ga_{0.47}As$ (001). In contrast to molecular beam epitaxy (MBE) grown $In_{0.53}Ga_{0.47}As(001)$, the STM results on decapped $In_{0.53}Ga_{0.47}As(001)$ do not show the existence of the heterodimer $In_{0.53}Ga_{0.47}As(001)$-(4×3) structure (4-5). At the intermediate annealing temperature ranges of 400 - 440°C, a (2×4)-(4×2) mixed surface reconstruction was observed. When $In_{0.53}Ga_{0.47}As(001)$/InP sample was annealed between 440°C and 470°C, a pure In/Ga–rich (4×2) surface reconstruction was observed.

Introduction

The integrated circuit (IC) industry has been geometrically scaling the physical dimension of complementary metal oxide semiconductor (CMOS) devices. Silicon based metal oxide semiconductor field effect transistor (MOSFET) technology may be approaching its theoretical physical limits (6-7). Therefore, the IC industry may need alternative materials to continue progress in device scaling. A group of materials that might provide a solution are III-V compound semiconductors because they exhibit ~5-20 times higher effective channel mobility, enabling much lower supply voltage (~0.5 V) than silicon (6-7). The key to fabricating a practical III-V MOSFET is forming an unpinned oxide-semiconductor interface with low fixed charge and low trap density (8). A high quality interface of oxide and III-V compound semiconductor has been found to be related to the semiconductor surface reconstruction (8-9).

$In_{0.53}Ga_{0.47}As$ is a convenient III-V compound semiconductor for a MOSFET channel material due to its high electronic mobility (~14,000 $cm^2 V^{-1} s^{-1}$), high breakdown field, and its ability to be grown lattice matched to a semi-insulator substrate, InP. Although GaAs(001) (2, 11) and InAs(001) (12-14) have been the focus of many scanning tunneling microscopy (STM) studies, very few STM studies of have been performed on $In_{0.53}Ga_{0.47}As(001)$ to understand and characterize the real space atomic surface structure (4-5). Millunchick *et al.* performed STM studies of three different In composition InGaAs(001) films, grown at a single temperature by molecular beam epitaxy (MBE) to identify the different As-rich surface reconstructions that were present on InGaAs(001). They found that the surface of $In_{0.53}Ga_{0.47}As$/InP(001) films has a heterodimer (4×3) [Fig. 1(a)] surface reconstruction, the surface of $In_{0.27}Ga_{0.73}As$/GaAs(001) films has a mixed heterodimer (4×3) and As-dimer α2(2×4)

[Fig. 1(b)] surface reconstruction, and the surface of $In_{0.81}Ga_{0.19}As$/InP(001) films has a mixed heterodimer (4×3) and As-dimer β2(2×4) [Fig. 1(c)] surface reconstruction (4).

The (4×3) surface reconstruction is dramatically different from the two (2×4) [α2(2×4) and β2(2×4)] reconstructions, which have similarities to each other. The (4×3) surface reconstruction has the unit cell which contains three Ga/In dimers and one heterodimer in the top layer along with one As dimer in the third layer [Fig. 1(a)]. Conversely, the (2×4) surface reconstructions, both have a top row of dimerized As atoms which are bonded to tricoordinated In/Ga atoms. Between the As rows are trough regions that contains one As dimer per unit cell. The main difference between the α2(2×4) and β2(2×4) structures is that α2 structure has single As dimer on the row [Fig 1(b)] and the β2 structure has double As dimers on the row [Fig 1(c)]. In addition, the α2 reconstruction has two degenerate reconstructions; the As dimer can either be on the left or the right of the row. This degeneracy causes the surface structure appears to have rows that are not completely straight in STM images.

In the present paper, the surface reconstructions of As-rich $In_{0.53}Ga_{0.47}As$(001)-(2×4) were further explored by STM using a decapping and annealing procedure over a range of temperatures. STM images of the $In_{0.53}Ga_{0.47}As$(001)-(2×4) showed that the surface contained the mixed single As-dimer α2(2×4) [Fig. 1(b)] and double As-dimer β2(2×4) [Fig. 1(c)] reconstruction, which density function theory (DFT) calculations (1-3) predict are stable for GaAs(001)-(2×4), InAs(001)-(2×4) and InGaAs(001)-(2×4) surfaces. As the annealing temperature was increased, the surface reconstruction of decapped $In_{0.53}Ga_{0.47}As$(001) changes to a (2×4)-(4×2) mixed reconstructions. For higher annealing temperatures, the surface reconstruction of decapped $In_{0.53}Ga_{0.47}As$(001) changes to the In/Ga-dimer (4×2) without a heterodimer (4×3) surface reconstruction.

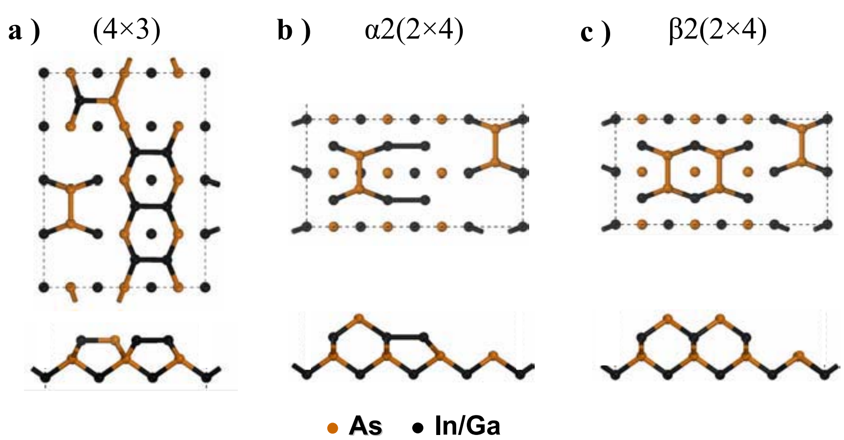

Figure 1. Top-down view of atomic structure with the cross sections for $In_{0.53}Ga_{0.47}As$(001)-(4×3) and (2×4) surface reconstructions: (a) (4×3) (4), (b) α2(2×4) and (c) β2(2×4).

Experimental Method

MBE was employed to grow 0.2 μm of 1×10^{18} cm^{-3} doped $In_{0.53}Ga_{0.47}As$ layer, lattice-matched to 500 μm thick InP(001) substrates with 1×10^{18} cm^{-3} doping. Experiments were performed on both *n*-type and *p*-type wafers. The re-grown wafers were capped in situ with a 50 nm protective arsenic cap. The wafers were transferred to a vacuum container for transporting to the STM chamber. The STM chamber is equipped with low energy electron diffraction (LEED) for confirmation of the surface periodicity and an Omicron VT STM.

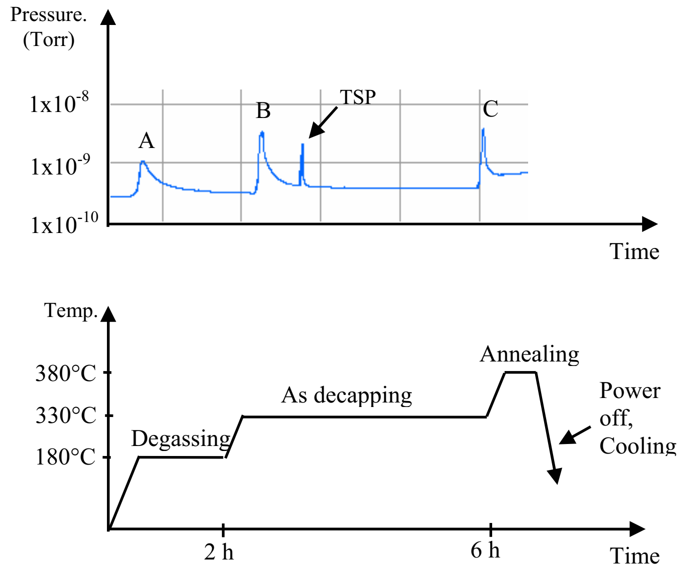

Figure 2. Example of $In_{0.53}Ga_{0.47}As$(001)-(2×4) sample decapping and annealing procedure showing the chamber pressure (blue line), program temperature (black line). Peaks A, B and C in the pressure plot correspond to pressure bursts due to degassing, arsenic decapping and high temperature annealing, respectively.

The As capped samples were radiatively heated to obtain the desired $In_{0.53}Ga_{0.47}As$(001) surface reconstruction. Figure 2 shows the temperature ramps and subsequent pressure rise during the preparation of $In_{0.53}Ga_{0.47}As$(001)-(2×4). A three step decapping and annealing procedure was performed. First, the samples were initially held at 180°C for at least 2 hours degassing. This removed the weakly bonded impurities from the surface such as water. Second, the sample temperature was raised to 330°C for typically between 2 and 4 hours. This removed the As-cap. Finally, the sample was gradually heated to the peak temperature following by quenching. The peak temperature determined the observed surface reconstruction. For example, $In_{0.53}Ga_{0.47}As$(001)-(2×4), mixed (2×4) and (4×2), and pure (4×2) surfaces were observed at 380°C, 400-440°C and 455°C peak temperatures.

Following the As-decapping and annealing procedure, the surface reconstruction was verified by LEED. Afterwards, the sample was transferred to the STM. STM images were taken at room temperature using constant-current mode with a tunneling current of 100 pA and sample bias voltage of -2 V relative to the etched tungsten tip.

Results and Discussions

The α2(2×4) and β2(2×4) are the most common reconstructions for III-V (2×4) surfaces. DFT calculations showed α2 and β2 structures are the stable reconstructions for GaAs(001)-(2×4) (1-2), InAs(001)-(2×4) (1) and $In_{0.53}Ga_{0.47}As$(001)-(2×4) (3) surfaces. The atomic models of α2(2×4) and β2(2×4) along with the Millunchick (4×3) model are schematically shown in Fig. 1. Figure 3(a) shows a filled state STM image of the clean $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface. To deduce the $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface reconstruction, the STM image was compared to filled state STM images of the

GaAs(001)-(2×4) [Fig. 3(b)] and InAs(001)-(2×4) surfaces [Fig. 3(c)]. The STM images show that the $In_{0.53}Ga_{0.47}As$(001)-(2×4) more closely resembles the InAs(001)-(2×4) than the GaAs(001)-(2×4). However, small regions of the $In_{0.53}Ga_{0.47}As$(001)-(2×4) image are similar to the GaAs(001)-(2×4) image.

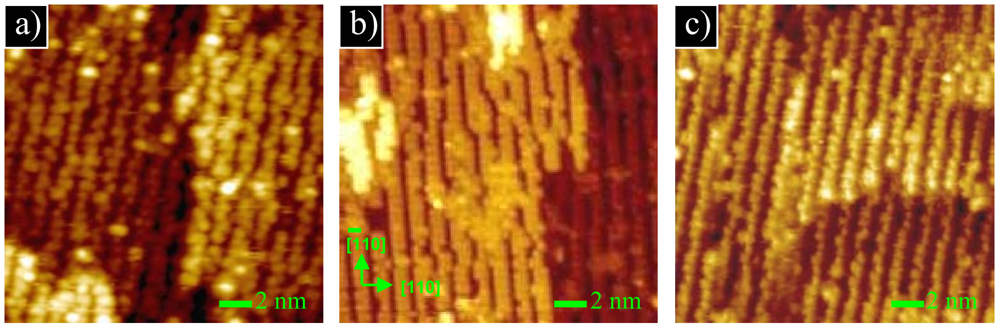

Figure 3. Filled state STM images (25 ×25 nm^2) obtained from clean (a) GaAs(001)-(2×4), (b) InAs(001)-(2×4) and (c) $In_{0.53}Ga_{0.47}As$(001)-(2×4) surfaces.

The GaAs(001)-(2×4) [Fig. 3(b)] surface has a nearly perfect β2(2×4) reconstruction with the exception of a few missing arsenic dimers that are caused by thermal desorption; this surface has been studied by many research groups (8, 15-16). The α2(2×4) surface reconstruction has never been observed on GaAs(001). However, DFT calculations predict that it is also a stable surface reconstruction for GaAs(001) (1). In comparison, the InAs(001)-(2×4) [Fig. 3(c)] surface is dominated by the α2(2×4) reconstruction with its zig-zagging rows. Although the current InAs(001)-(2×4) surface is made up almost entirely of α2(2×4), if the annealing temperature is decreased, an increasing amount of β2(2×4) areas will be observed on the surface. The β2(2×4) reconstruction which has a double top As dimers row was observed by Ratsch *et al.* under As rich conditions on InAs(001) grown by in situ MBE (1). The $In_{0.53}Ga_{0.47}As$(001)-(2×4) [Fig. 3(a)] surface exhibits zig-zagging rows which is indicative of α2(2×4) reconstruction. However, there is a 2 to 4 times higher faction of double As-dimers on the row of $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface than on the row of InAs(001)-(2×4) based on the current STM images.

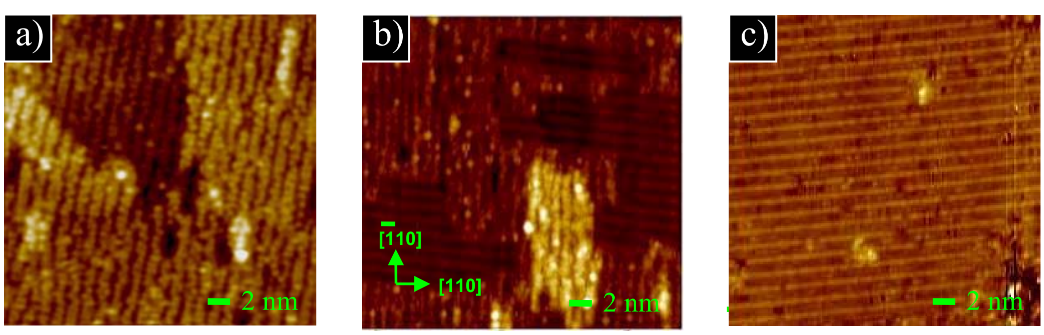

Figure 4. STM images obtained from clean $In_{0.53}Ga_{0.47}As$(001) annealed at (a) 380°C As-rich (2×4), (b) 437°C mixed (2×4)-(4×2), and (c) 455°C group III-rich (4×2).

The surface reconstructions were investigated on $In_{0.53}Ga_{0.47}As$(001)/InP as a function of the substrate temperature. There are three temperature regimes: (i) low temperature 330-400°C, (ii) intermediate temperature 400-440°C and (iii) high temperature 440-470°C. (i) When the sample was annealed between 330°C (As decapping temperature) and 400°C, the As-dimer (2×4) reconstruction was observed. As shown in Fig. (4a), the As rich- $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface structure is primarily made up of α2(2×4) with small regions of β2(2×4). The optimal temperature for preparing $In_{0.53}Ga_{0.47}As$(001)-(2×4) is 380°C. (ii) When the sample annealing temperature was between 400-440°C, a mixed as-dimer (2×4)/(4×2) reconstruction was observed without any regions of the heterodimer (4×3). It is possible that the heterodimer (4×3) regions can only be generated by in situ MBE which allows control of As flux as well as surface temperature. As shown in Fig 4(b), the (2×4) terraces are a monolayer step above the (4×2) terraces. The same mixed surface reconstruction has been previously reported for InAs(001) surface (17), but this mixed (2×4)/(4×2) surface structure has never been observed in GaAs(001). (iii) When the sample was annealed between 440°C and 470°C, the In/Ga dimer $In_{0.53}Ga_{0.47}As$(001)-(4×2) surface reconstruction was observed. As shown in Figure 4(c) the (4x2) surface has an In/Ga dimer (4×2) reconstruction across the entire surface. The clean $In_{0.53}Ga_{0.47}As$(001)-(4×2) surface was found to closely resemble the InAs(001)-(4×2) surface and was dissimilar to well documented the GaAs(001)-ζ(4×2) surface (2). Details of the GaAs(001)-(4×2), InAs(001)-(4×2) and $In_{0.53}Ga_{0.47}As$(001)-(4×2) have been discussed elsewhere (18-19). Heating above 470°C induces surface disorder probably from depletion of As from the bulk.

Summary

In conclusion, high resolution STM images of the decapped $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface reconstruction have been obtained. The (2×4) surface reconstruction is dominated by α2(2×4) structure, which contains zig-zagging row features in the STM images. However, there is a 2 to 4× higher fraction of double As dimers on the rows of the $In_{0.53}Ga_{0.47}As$(001)-(2×4) surface than on the rows of the InAs(001)-(2×4) surface. The surface reconstruction of decapped $In_{0.53}Ga_{0.47}As$(001)/InP changes with increasing annealing temperature first to a mixed (2×4)-(4×2) surface reconstruction between 400 - 440°C and finally to a pure In/Ga dimer (4×2) structure for temperatures in excess of 440°C.

Acknowledgments

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