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Ga-induced restructuring of Si(5 5 12) − 2 × 1 reconstructed surface at room temperature

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ABSTRACT

Motivated by the need to form 1D-nanostructured dopants on silicon surfaces, we have attempted to grow Ga on the high index Si(5 5 12) surface which has a highly trenched (1D) morphology. The evolution of the interface with Ga adsorption in the monolayer regime has been probed by in situ AES, LEED and EELS. Controlling the kinetics by changing the Ga flux rates shows an interesting difference in the 1.0 to 1.5 ML region. The low flux rate (0.03 ML/minute) results in a Frank van der Merwe (layer by layer) growth mode up to 2 ML, while the higher flux rate (0.1 ML/minute) shows a transient island formation after the completion of 1 ML. The low rate shows the formation of 2 × (3 3 7) and (2 2 5) superstructures, while only the 2 × (3 3 7) is observed in a wide coverage range for the higher rate. The results demonstrate the ability to kinetically control the surface phases with different electronic properties of this technologically important interface.

1. Introduction

Recent interest in the growth of metals on various low and high index silicon surfaces is motivated by the needs to find suitable templates for self-assembled nanostructure formation [1–3], whose exotic low dimensional properties can be used to develop advanced devices such as single-electron transistors, quantum dot laser, HB LEDs etc. [4,5]. Forming buried nanostructures of dopant metal silicon can have great implications in devices of the future [6]. The contemporary challenges in nanoscale device fabrication require feasibility in fabrication and also an understanding of the fundamental physical and chemical processes involved [7,8]. In order to grow such self-assembled nanostructures on a large scale and apply them to nano-devices of high density, a well-defined template at the nanometer scale should be prepared. One of the potential substrates to satisfy these goals to form 1D structures is the high index Si(5 5 12) − 2 × 1 surface with a large unit cell of 5.35 × 0.77 nm^2, since it is reconstructed to a planar surface having single domain grooves with one-dimensional (1D) symmetry [9]. In literature several atomic models of Si(5 5 12) have already been determined by using different surface sensitive techniques [10–13], after it was discovered by Baski et al. [14]. A consensus now exists that, on the reconstructed Si(5 5 12) − 2 × 1 surface, a chain structure divides each (5 5 12) unit into two (3 3 7) and one (2 2 5) subunits [15] in whose vicinity there are several (h k l) planes, and thus upon metal adsorption, subtle energetic changes can result in faceting [16]. Studies of the adsorption of a few metals on Si(5 5 12) and other high index Si surfaces such as (3 3 7), (1 1 2) etc. have already been reported in literature [17–26], revealing the formation of 1D and 2D nanostructures with large aspect ratio. More specifically, adsorption of Ga on high index Si surface has attracted great attention because of the surge in activities related to the formation of GaN based optoelectronic devices on Si surfaces. Ga adsorption on high index Si surfaces such as (1 1 2), (5 5 3), (5 5 7) etc. has already been reported in literature, such as Baski et al. [27], who have studied the adsorption of Ga on Si(1 1 2) and (3 3 7) and concluded that these particular high index surfaces facet to other orientations depending on the kinetics of Ga adatoms. Si(1 1 2) reconstructs into (1 1 1) and (3 3 7), while Si(3 3 7) transforms into (5 5 12) with different Ga coverage. Erwin et al. [28] have addressed the issue related to vacancy-line interaction on Ga/Si(1 1 2) interface. In another report Baski et al. [29] and Schimdt et al. [30] have shown the Ga induced 5 × 1 and 6 × 1 on Si(1 1 2) surface. However, to the best of our knowledge there is no report yet on the Ga/Si(5 5 12) interfacial system in literature.

In this work, we report the first time study of the Ga (Gp-III acceptor) adsorption on Si(5 5 12) − 2 × 1 reconstructed surface at room temperature (RT) and demonstrate the subtle kinetic effect for two different Ga flux rates. The Ga flux rate can influence the diffusion of adsorbate and consequently the nucleation density and growth mode. The Ga/Si(5 5 12) interface evolution has been probed by *in-situ* surface sensitive techniques such as Auger Electron Spectroscopy (AES), Low Energy Electron diffraction (LEED) and Electron Energy Loss Spectroscopy (EELS). The results have led us to extract a 2D-phase diagram for this system and monitor the interface evolution.

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2. Experimental

The experiments were performed *in-situ* in an UHV chamber, with a base pressure of better than 5×10^{-11} Torr equipped with a high precision sample manipulator, a Cylindrical Mass Analyzer (CMA) with a resolution of 0.18% with a concentric 0–10 kV electron gun to perform AES and EELS, and a four grid optics for LEED studies. The sample is a $20\times5mm^2$ piece cut from a p-type boron doped Si (5 5 12) wafer having a resistivity of 10–15 Ω-cm. The sample was cleaned by the modified Shiraki process [31] before inserting in the vacuum chamber and mounted onto the high-precision manipulator with homemade Ta sample holder. After inserting into the vacuum chamber, the sample is degassed at 600 °C by direct resistive heating for 12 hours followed by repeated flashing up to 1200 °C for 5 seconds and cooling to RT at a very slow rate of 2 °C/second [32]. The sample temperature is monitored by a W-Re (5%, 25%) thermocouple mounted behind the sample that is calibrated by an optical pyrometer. The atomic cleanliness of the sample was ascertained by the absence of carbon and other contaminants on the surface by AES and by the observation of the characteristic LEED pattern of the (2×1) reconstruction of the Si(5 5 12) surface. Gallium deposition was made from a homemade tantalum-Knudsen cell, which was degassed properly before evaporation. The flux rate was controlled by regulating the current to the cell and is measured in terms of the adsorbed monolayer (ML) per unit time by measuring the Ga (MNN) to Si (LVV) Auger peak intensity ratio. A monolayer is defined as 6.8×10^{14} atoms/cm^2, which is the bulk truncated surface atomic density of the Si (5 5 12) surface. The AES, EELS spectra and the LEED pattern were digitally acquired and analyzed at every incremental adsorption of Ga on Si(5 5 12) surface at RT.

3. Results and discussions

Ga adsorption has been performed at two different flux rates on the 2×1 reconstructed Si(5 5 12) surface, while the substrate is at room temperature (RT). The Ga uptake curve in Fig. 1 shows the plot of the intensity ratio of the Ga (LMM) at 55 eV to Si(LVV) at 92 eV Auger peaks, as a function of deposition time for the two deposition rates LFR and HFR (quantified later). Curve (a) shows increase in the Auger intensity ratio up to 66 minutes of Ga adsorption, with a change in slope at 33 minutes. To precisely determine the break point at 33 minutes, we adopt the SSQ (sum of squares of error) method [33], which has been plotted as the dotted curve in Fig. 1. This break in slope of the curve is attributed to the beginning of the attenuation of Auger signal from first layer by the second layer adatoms and thus provides a calibration for 1 ML coverage, yielding a Ga flux rate of 0.03 ML/minute (Low Flux Rate—LFR). After 66 minutes of Ga adsorption, we have observed saturation in the Auger intensity ratio, which can be attributed to the formation of 3D islands. Overall, curve (a) shows the characteristic behavior of Stranski–Krastnov (SK) where islands form after 2 ML of layer by layer Ga adsorption. For curve 1b, we have observed an interesting change, which shows a linear increase in the Ga/Si Auger intensity ratio up to 10 minutes of Ga adsorption (alternate *X*-axis) after which it saturates upon 15 minutes of Ga adsorption, yielding a flux rate of 0.1 ML/minute (High Flux Rate—HFR). Normalizing the *X*-axis to the saturation values of the ratios in both LFR and HFR (2 ML), we observe deviation of curve b (HFR) from curve a (LFR), due to a brief flattening in the 10- to 15-minute range, which suggests that for the HFR case, there is a deviation from Frank van der Merwe mode. This can be attributed to the formation of 3D islands on top of 1ML of Ga adsorption. After 15 minutes of Ga adsorption, Auger intensity ratio again starts increasing steeply up to 20 minutes of Ga adsorption, where it attains a value of 0.34 (corresponding to 2 ML of Ga) and saturates. This indicates that after a complete monolayer of Ga adsorption, initially Ga grows as large 3D island, and with further increase in coverage (>1.5 ML) these 3D islands re-convert into 2D layers. We have recently reported on such clustering and layering phenomena observed at the In/Si(111) interface [23]. It is important to recollect here that Ga adsorption at this flux rate (0.1 ML/minute) on low index Si(111)-7×7 reconstructed surface [34,35] shows no 3D island formation after 1 ML of Ga adsorption. This difference in the growth mechanism can be attributed to the difference in the kinetics of adsorbed Ga monomers. The higher rate promotes early nucleation and 3D island formation, while the lower flux provides sufficient time for Ga adatoms to bind at appropriate 2D sites, thus minimizing the dangling bond density, in a low strained configuration. The figure also shows the different phases observed with the Ga coverage for both LFR and HFR Ga adsorption at room temperature.

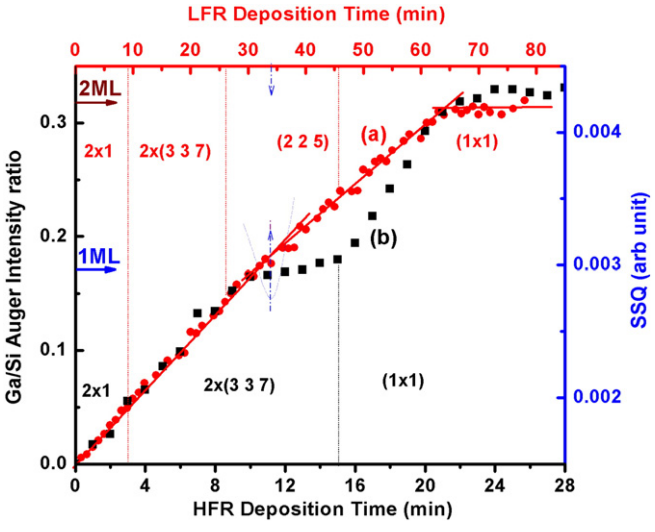

Fig. 1. Shows the Ga uptake curve on Si(5 5 12) surface at RT, by plotting the Si(LVV) to Ga(LMM) Auger intensity ratio versus the deposition time. Curve (a) shows the uptake curve for Ga flux rate of 0.03 ML/minute, while curve (b) corresponds to 0.1 ML/minute. Various vertical lines show the surface phases observed by LEED for LFR and HFR, above and below the uptake curves, respectively. Also shown by the dotted curve is the SSQ to determine 1.0 ML break.

In order to identify the evolution of the superstructural phases during Ga adsorption at different flux rates on Si(5 5 12) -2×1 reconstructed surface, LEED studies have been carried out at different primary beam energies after each Ga adsorption. (i), (ii) and (iii) in Fig. 2 correspond to the LEED pattern, its line scan (along the [6 6 $\bar{5}$] direction) and its schematic, respectively. The intensity of the bulk related spots in the line scan in Fig. 2(ii) has been marked with down arrows, and the unit cell distances of the phases are calculated with respect to them. The fractional order spots of LEED are indicated by the two dotted lines in the same line scan, while the unit cell distance along the [6 6 $\bar{5}$] direction is marked by two horizontal arrows. Fig. 2(a) shows the LEED pattern of the clean Si(5 5 12) -2×1 reconstructed surface, which consists of sixteen equally spaced spots. The weak streaks seen parallel to the intense line of spots along the [6 6 $\bar{5}$] direction manifests the 2×1 reconstruction of Si(5 5 12) surface along the [$\bar{1}$ 1 0] direction. The distance between two consecutive fractional order spots along the [6 6 $\bar{5}$] direction, as calculated from the line scan, gives the distance of the wide unit cell of Si(5 5 12) oriented surface to be 1.17 nm^{-1} (5.35 nm in real space), where as the weak streak along [$\bar{1}$ 1 0] direction gives the other unit cell distance of 0.762 nm^{-1} (8.24 nm in real space). For the LFR case, when Ga adsorbs on Si(5 5 12) surface at RT, the spots weaken in intensity and the weak streaks of the 2×1 reconstruction in the [$\bar{1}$ 1 0] direction are lifted after 0.2 ML of Ga adsorption, yielding the bulk (1×1) structure. This indicates the formation of Ga induced surface symmetry of bulk truncated Si(5 5 12) along [$\bar{1}$ 1 0] direction, i.e., 0.38 nm^{-1} up to the coverage of <0.3 ML. As the Ga coverage attains 0.3 ML the weak LEED pattern transforms to an ordered structure as shown in Fig. 2(b)