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Higher order reconstructions of the Ge(001) surface induced by a Ba layer

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ABSTRACT

Structural properties of Ba-induced reconstructions on a Ge(001) surface, based on atomic-resolution ultra high-vacuum scanning tunneling microscopy measurements, are discussed. It is shown that while the Ba - Ge layer, which fully covers the surface, is dominated by a phase with an internal 2×3 periodicity, it also includes portions of higher order 2×6 and 4×3 surface reconstructions, always accompanied by 1D protrusions embedded into the dominating phase. Modelling the observed higher order structures, using the elementary cell of the 2×3 phase calculated within the density functional theory, is shown to reproduce the experimental data very well. As such the higher order reconstructions can be treated as local defects of the dominating 2×3 phase.

1. Introduction

The Si(001) and Ge(001) surfaces are known to be prone to the adsorption of residual gases in ultra-high vacuum (UHV) conditions. On the Ge(001) surface, for example, this leads to the formation of unwanted, disordered amorphous oxide, see e.g. [1,2]. One way to protect the (001) substrates of Si and Ge from this type of adsorption is to cover them with a monoatomic passivating layer [3,4]. The chemisorption of atomic hydrogen is a typical example [5–7], however, deposition of the alkali earth metals on Si(001) and Ge(001), that promotes the growth of a two-dimensional continuous passivating monolayer, is technologically more relevant [3,8–17].

Ultra-high vacuum scanning tunneling microscopy (UHV STM) investigations demonstrated that the deposition of 1/3 ML Ba on the Si(001) substrate, kept at 1170 K during and after processing, lead to the 2×3 surface reconstruction of the formed passivating adlayer [8]. The same technique was used in Ref. [9] to investigate room temperature (RT) adsorption of Ba atoms on Si(001) followed by annealing at 1160 K [9]. The 2×3 reconstruction was found to be formed at ~1/3 ML coverage of Ba along with local $c(2 \times 6)$ reconstructions. The authors suggested that the Ba-induced 2×3 periodicity could be created by the substitution of three neighboring Si surface dimers by one Ba dimer in the same Si dimer row [8,9]. Modified model, consists of single Ge dimer and one alkaline earth metal atom creating the surface unit cell, supported by the density functional theory (DFT) calculations, explains very well the observed 2×3 and 2×6 reconstructions for the Sr/Si(001) [11,18,19] and the Ba/Si(001) systems [20].

Incorporation of the Na atoms into the Ge(001) $c(4 \times 2)$ reconstructed surface at higher temperatures leads to the formation of global 2×3 and 6×3 structures, induced by 1/6 ML and below 0.1 ML of the Na residual coverage, respectively [16,17]. Adsorption of Sr and Ba on Ge(001) at elevated temperatures and different

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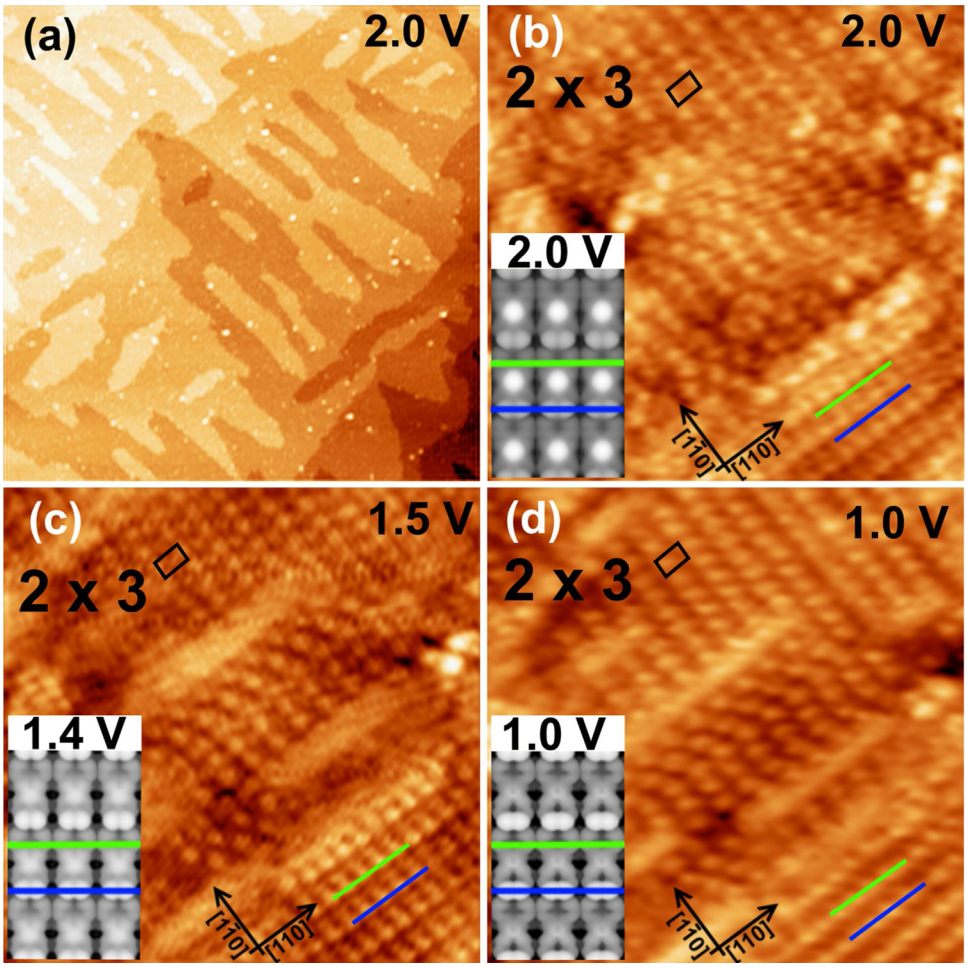

Fig. 1. Empty state STM images of the Ba ad-layer created at the Ge(001) surface. (a) Large-scale ($400 \times 400\ nm^2$) image taken after the deposition of 0.4 ML Ba on Ge(001) followed by annealing to 920 K (STM tunneling current $I_T = 20$ pA, sample bias voltage U = 2.0 V). (b– d) images of the same $20 \times 20\ nm^2$ area of the surface, obtained at different sample biases. Domains with a predominant 2×3 order are clearly visible at the same positions, marked by green and blue lines. Insets represents simulated STM images obtained by multiplication of the previously calculated individual 2×3 unit cell [23]. All images taken at 100 K (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

coverages was reported by Lukanov et al. [12–14]. They observed, depending on coverage, a number of distinct surface reconstructions including 2×3, 4×3, 9×1 and 6×1. Also, parallel, atomically flat structures alternated with narrow trenches were found to be formed from adsoption of both the Sr and Ba adatoms [12,13,15]. Details of the Sr-induced 4×3 structure on Ge(001) were studied experimentally and theoretically by the same group [13]. The proposed structural model for this reconstruction was based on a modified version of the Sr-induced 2×3 structure on Si(001). The model was successfully verified experimentally (UHV STM studies) and theoretically (DFT calculations) by Reiner et al. [18,22].

It has been predicted that the formation of continuous monolayers of Sr or Ba on Ge(001) leads to compressive surface strain [12]. This strain, presumably associated with the covalent radii of alkaline earth metal atoms being larger than those of the Ge atoms [14,15], results in higher mobility of the Ge dimers, large scale surface structural rearrangements and the formation of surface alloys, after annealing the samples at higher temperature (1070 K). This process also leads to the formation of non-uniform plateaus (stripes) of the Ba/Ge(001) phase with monoatomic height [3,15].

In this paper we discuss atomic-resolution STM data for the Ba/Ge(001) plateaus with predominantly long-range 2×3 periodicity interrupted by inserts with 2×6 and 4×3 orders. We provide a qualitative explanation of the reported observations, based on the structural models for the 2×3, $c(2 \times 6)$ and 4×3 surface reconstructions constructed using the elementary unit cell calculated for the defect-free 2×3 Ba/Ge(001) system [23]. We also report the formation of one dimensional (1D) protrusions, of up to several nanometers in length, that usually accompany the Ba induced reconstructions and are typically observed at boundaries between different Ba-induced surface phases, regardless of the preparation procedure.

2. Methodology

The study was carried out in ultra-high vacuum (UHV) conditions with a base pressure of $\sim 7 \times 10^{-11}$ mbar. The UHV system was equipped with a variable temperature Omicron VT STM XA head. An ion gun, evaporators, a heating stage and other preparation tools were mounted inside a separate, preparation chamber connected to the UHV system.

The Ge(001) substrates were cut from a commercially available Sb-doped wafer. The 3 mm × 8 mm samples were mounted on a standard direct-current heating sample holder. A clean reconstructed Ge(001) surface was prepared by a few cycles of annealing the sample at 970 K in UHV conditions, followed by Ar^+ ion sputtering with an energy of 0.75 keV [15,24]. A Ba atom beam was generated with a commercial Focus EFM-3 electron beam evaporator (acceleration voltage 500 V) from the Mo crucible.

We studied the Ge(001) sample with 0.4 ML of Ba deposited at room temperature (RT). The 0.4 ML Ba/Ge(001) sample was sequentially annealed at 620 K, 720 K (both for 30 min), 820 K and 920 K (both for 10 min). The Ba coverage, defined as the ratio of the number of Ba adatom to the number surface Ge atoms, was estimated using the coverage dependence on deposition parameters (cf. flux current, exposition time), as in our previous STM study [21]. The temperature of the substrate was measured with a thermocouple, held in contact with the sample holder, close to the sample, and by an external pyrometer (for temperatures above 770 K). The STM images were taken at 100 K, using electrochemically etched tungsten tips. The WSxM software was used for data processing [25].

3. Results and discussion

Fig. 1 shows the STM images of the Ba-Ge intermixed phase as a result of the RT deposition of 0.4 ML Ba on the clean Ge(001) c(4 × 2) reconstructed surface, followed by sequential annealing up to 920 K. A similar surface morphology was reported on Ge(001) for larger (1 ML) initial Ba coverage after annealing at a higher temperature (1070 K) [15].

The representative large-scale STM image of the adsorbed surface shown in Fig.1(a) reveals the presence of elongated stripes or islands of mono-atomic adlayer plateaus of apparent height 0.14 ± 0.05 nm (measured at a sample bias voltage of + 2.0 V). It should be noted that the observed plateaus do not reproduce typical shapes of the terraces observed on clean Ge(001) c(4 × 2), see e.g. [24]. Also, the stripes and islands are wider than that observed in the Sr/Si(001) and Na/Ge(001) systems [12,16,17]. The presence of wider stripes on the Ba/Ge(001) surface suggests that the Ba-induced islands are less strained that those formed by Sr on Si(001) [26] and by Na on Ge(001) [17]. It is also noteworthy that the Ba adstructures on Ge(001) were obtained at lower temperatures (920 K) than those on Si(001), which were formed at ∼1160 K [8,9].

The enlarged areas of the 0.4 ML Ba/Ge(001) sample are displayed in the empty state STM images of Fig.1b–d (bias voltages of 2.0 V, 1.5 V and 1.0 V, respectively) and reveal structural details of the Ba adlayer. Firstly we observe that the dimerized clean Ge(001) surface is not visible, i.e., the surface is fully covered by the Ba monolayer. Secondly, the imaged stripes consist of separate rows of linearly ordered bright circular protrusions that form a regular 2D lattice with a rectangular unit cells. This lattice has a 2 × 3 periodicity and dominates the Ba covered Ge(001) surface This 2 × 3 phase was also observed in previous experimental studies on Ba incorporated into the Ge(001) [3,15,23] and Si(001) substrates [8,9], and Sr or Na intermixing with the surface atoms of Si(001) and Ge(001) [10–12,17].

Close inspection of the bias dependent images of Fig. 1b-d shows that each individual protrusion consist of two components which are separated by about 0.4 nm (size of the elementary surface unit cell of the clean Ge substrate [27]) along the [1–10] (or [110]) surface directions, see Fig. 2. In addition, the relative intensity of these components changes with the bias voltages. We observe that the brighter component imaged at high bias voltage (2 V – Fig. 1b) becomes darker when imaged at low bias voltage (1 V – Fig. 1d) – for example note the protrusions between two lines (green and blue) placed in equivalent positions in Fig. 1b–d. This sequence reverses for the second component of the protrusion. At the intermediate bias voltage (1.5 V, Fig. 1c) both components in the protrusion have a similar brightness. No such bias dependence has been observed in the corresponding filled state STM images.

In order to elucidate the observed behavior we consider simulated STM images of the elementary 2 × 3 cell, calculated using the density functional theory (DFT) and the Tersoff-Hammann approximation [28] (see Ref. [23] for details). The accepted model for the 2 × 3 unit cell contains one Ba adatom (substituting two Ge dimers in the most top Ge layer) and a single Ge dimer between neighboring Ba atoms along the [110] surface direction [18,22,23] – see Fig. 2. The calculations for the intermediate bias voltage (1.4–1.5 V) shown in Fig. 2 reveal that the protrusions in the imaged pair are attributed to the Ge surface dimer (brighter) and to the Ba incorporated atom (darker). It follows that the brighter components seen at the high bias voltage (2.0 V - Fig. 1d) represent the incorporated Ba dimers and that at the low bias voltage (1.0 V Fig. 1b) the brighter components represent the surface Ge dimers. The simulated, bias dependent STM images are also incorporated into the corresponding experimental STM images (see the insets in Fig. 1b–d). Also, to make sure that one looks at the same areas in both the experimental and simulated STM images, two lines (green and blue) are placed in equivalent positions in both images.

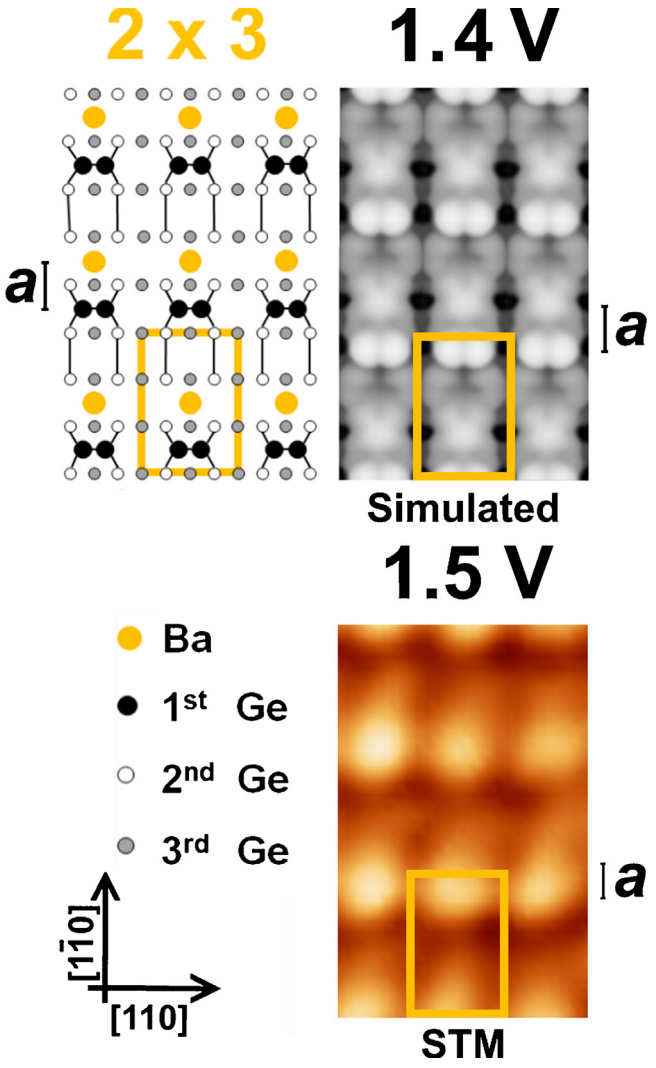

Fig. 2. Ball-and-stick model of the 2 × 3 surface structure compared with the DFT simulation for bias voltage 1.4 V and STM image recorded at 1.5 V (2.4 × 3.6 nm^2), respectively. The elementary 2 × 3 unit cell is marked as a yellow rectangle. The size of the unit cell of the clean Ge(001) substrate (a) is also shown in each figure (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

The higher order reconstructions that are observed as embedded into the dominating 2 × 3 reconstruction are shown in the empty state images (1.5 V) of Fig. 3. The chosen value of the bias voltage allows simultaneous observation of the Ba atom and Ge surface dimers. It is observed (Fig. 3a) that there are two distinct domains

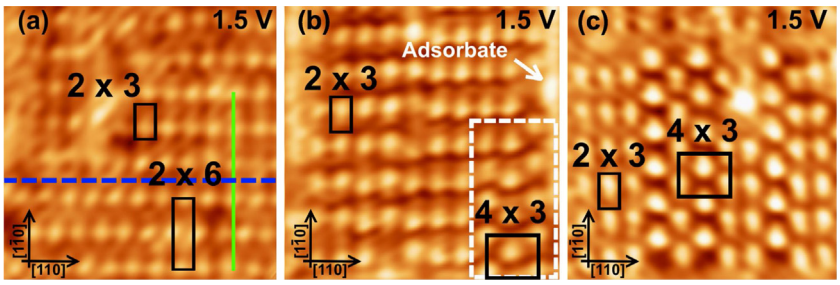

Fig. 3. Representative empty state STM images of the Ba/Ge(001) surface of 10 nm × 10 nm area (measured with I_T = 120 pA), and processed with a FFT filter. (a) shows the 2 × 3 and 2 × 6 phases (above and below the dashed line, respectively). The green line indicates the [1–10] direction in the 2 × 3 structure and helps to observe the shift in the [110] direction of protrusions in alternate rows in the lower domain). (b) the black rectangles mark 2 × 3 and 4 × 3 unit cells; the dashed-line rectangle indicates formation of the 4 × 3 domain emended within the 2 × 3 phase near an adsorbate; (c) area with the 4 × 3 domains surrounded by the 2 × 3 phase on the narrow plateaus (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

of different order visible above and below the horizontal dashed line. The difference between the upper and lower domains is clearly visible by highlighting the [1–10] direction marked by the green line in Fig. 3a. One observes that in the upper part (2 × 3 phase) the bright protrusions lie along the green line, while in the lower part (2 × 6 phase) the green line crosses the protrusions located on every second row. The upper domain has the 2 × 3 periodicity with the corresponding rectangle unit cell. The lower domain represents a phase with a 2 × 6 periodicity with the unit cell marked by an elongated rectangle.

Fig. 3b and c show the second higher order reconstruction - 4 × 3 - observed within the Ba induced 2 × 3 phase on Ge(001). In Fig. 2b the region dominated by the 4 × 3 phase is contained within the dashed (white) rectangle. A different arrangement in which the 4 × 3 domain is interfaced with the 2 × 3 phase, is shown in Fig. 3c. Two narrow regions of the 4 × 3 phase are surrounded by 2 × 3 phase - the one on the left is two unit cells wide (with the right unit cell indicated), and the one on the right is one unit cell wide.

Fig. 4 shows the schematics of the 2 × 6 and 4 × 3 phases. It appears that both can be composed based on the elementary unit cells of the 2 × 3 phase. The 2 × 6 structure can be formed by shifting every second row of a 2D - 2 × 3 lattice by half of the size of the unit cell of the Ge substrate in the [110] surface direction (compare Figs. 2 and 4a) and the 4 × 3 domain can arise by shifting every second row by half of the unit cell size in the [110] direction, including a mirror reflection of the shifted row (compare Figs. 2 and 4b). The corresponding simulated STM images (bias 1.4 V) are also shown in Fig. 4. The STM images are composed based on the elementary unit cell of the 2 × 3 phase, calculated within DFT [23], into the corresponding 2D lattice of the 2 × 6 and 4 × 3 periodicities. The STM data (bias 1.5 V) presented in the Fig. 3 are in a good agreement with the models in Fig. 4. indicating that the higher order reconstructions can be treated as local, spatially extended defects within the dominating 2 × 3 phase. We would like to note that all observed Ba-induced surface structures correspond to the 1/6 ML theoretical concentration of the Ba atoms on the surface.

One more structure that has commonly been observed on the Ba/Ge(001) – 2 × 3 reconstructed surface is a 1D protrusion shown in Fig. 5. These protrusions are randomly distributed on the surface, often isolated from the surrounding structure of the same apparent height – see (i) in Fig. 5a - but sometimes appear to emanate from the edge of a terrace – see (ii) in Fig. 5a. Close inspection of the STM images shown in Fig. 5b, and c demonstrate that the 1D protrusions share several common properties: (1) the surface of the 1D structures appears uniform with no internal, atomically resolved features, even though the terrace structures are imaged with atomic resolution in the empty state images; (2) their appearance does not strongly change with imaging conditions; (3) they are located directly on the dominating protrusion of the 2 × 3 reconstruction at positive bias STM imaging and align with the most top layer Ge surface dimer; (4) the apparent height of individual 1D protrusions is approximately the same as that of the upper level of the ordered Ba-induced protrusions observed in empty state STM imaging and higher about 30 - 60 pm in the filled state images; (5) their position does not vary with scan and imaging parameters; (7) their length varies from approximately 3 nm to over 20 nm and they are frequently connected with the neighboring edge of plateaus.

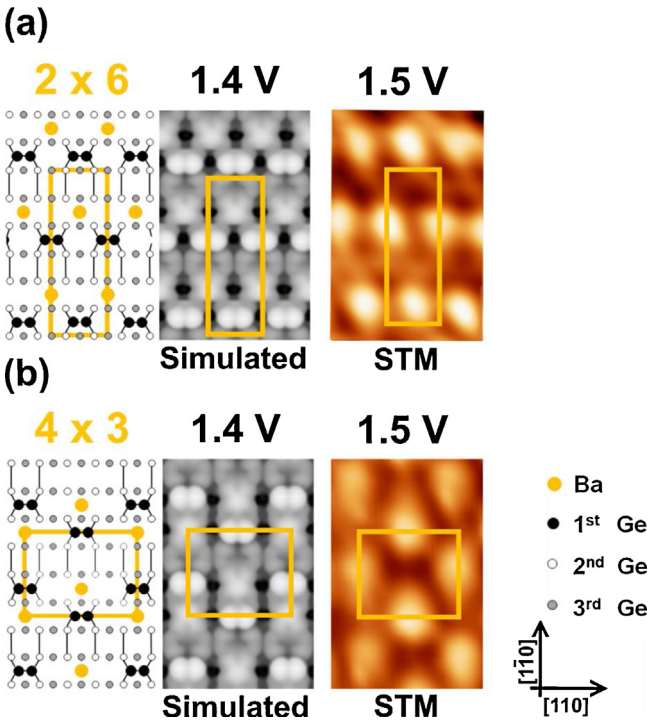

Fig. 4. Structural models of (a) 2 × 6 and (b) 4 × 3 phases for the Ba ad-layer on Ge(001). The models are based on the predictions made for the Sr/Si(001) and Sr/Ge(001) systems [13,18,22], and adopted for the Ba/Ge(001) structure [23]. The simulated STM images are compared with corresponding experimental STM images (areas of 2.4 × 3.6 nm^2) recorded at 1.5 V bias voltage (see text for details).

Based on the models presented in the Figs. 2 and 4 it can be concluded that these 1D protrusions represent the native, top-most layer of Ge dimer rows which do not interact with Ba atoms. This seems to be supported by the observations that they are exclusively detected within the 2 × 3 phase. This is also in line with Ref. [20] where very similar structures were observed in the Ba/Si(001) system and identified as Ge surface dimer rows. In addition, in the p(6 × 3) phase,observed for the Na/Ge(001), the Na chains are separated by the Ge top layer dimer rows and these rows exhibit

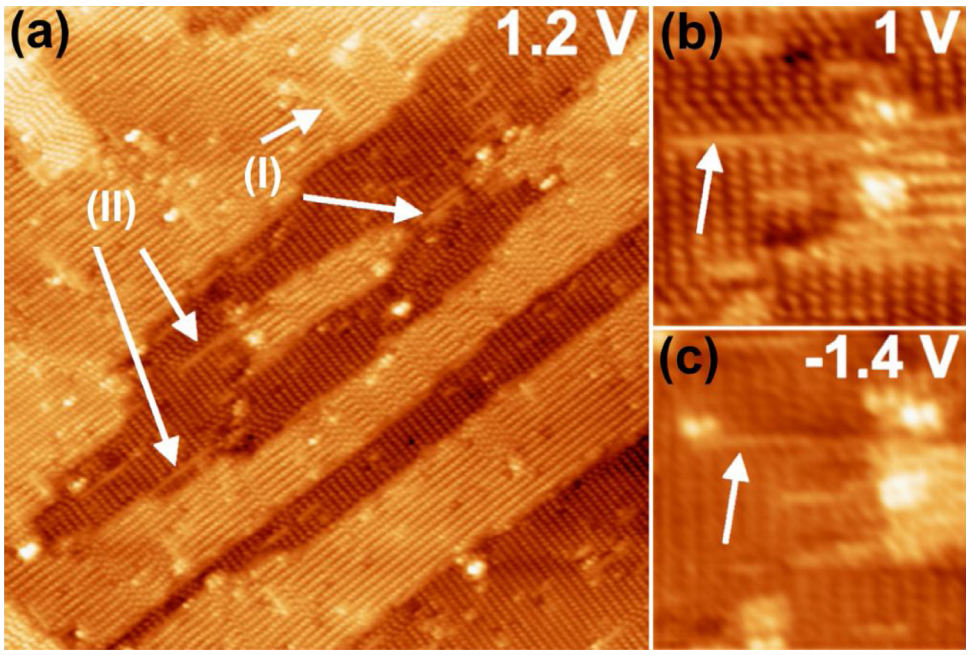

Fig. 5. STM images of the reconstructed Ba/Ge(001) surface. (a) 100×100 nm^2 region of the sample with the initial coverage 0.4 ML annealed sequentially up to 920 K, with the dominating protrusion of the Ba induced structure visible, along with frequent 1D protrusions; (c) and (d) enlarged images of same area (20×20 nm^2) imaged at empty and filled states, respectively. White arrows indicate positions of 1D protrusions.

similar topographical properties to the 1D protrusions observed in our experiments [16].

4. Summary

We have analyzed the atomic structure of the Ba/Ge(001) adsorption system. The study has led us to the following conclusions: (1) the 2×3 reconstruction is the dominant surface phase induced by Ba and other alkaline earth metals on the Ge(001) surface; (2) domains formed in a monolayer of Ba/Ge monolayer on the Ge(001) surface at elevated temperatures can contain areas of local higher-index (2×6 and 4×3) surface structures. While such reconstructions have already been observed in the incorporation phases of alkaline earth metals on the Si(001) substrate, they have not observed on the Ba/Ge(001) surface; (3) the structural properties of the higher order phases indicate that they can be composed from the 2×3 unit cells and as such represent surface defects in the uniform 2×3 phase; (4) frequently observed 1D protrusions, located in the otherwise 2×3 ordered two-dimensional regular Ba lattice, are consistent with those seen in the Ba/Si(001) (there they are identified as Ge surface dimer rows), however their unambiguous identification as either being composed of adatoms of Ge, Ba or both, is yet to be confirmed.

Acknowledgments

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