# Electronic and energetic properties of Ge(110) pentagons

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## ARTICLE INFO

## ABSTRACT

The electronic and energetic properties of the elementary building block, i.e. a five-membered atom ring (pentagon), of the Ge(110) surface was studied by scanning tunneling microscopy and spectroscopy at room temperature. The Ge(110) surface is composed of three types of domains: two ordered domains (($16 \times 2$) and c($8 \times 10$)) and a disordered domain. The elementary building block of all three domains is a pentagon. Scanning tunneling spectra recorded on the ($16 \times 2$), c($8 \times 10$) and disordered domains are very similar and reveal three well-defined electronic states. Two electronic states are located at 1.1 eV and 0.3 eV below the Fermi level respectively, whereas the third electronic state is located at 0.4 eV above the Fermi level. The electronic states at $-0.3$ eV and 0.4 eV can be ascribed to the pentagons, whilst we tentatively assigned the electronic state at $-1.1$ eV to a Ge–Ge back bond or trough state. In addition, we have analyzed the straight $[1\bar{1}2]$ oriented step edges. From the kink density and kink–kink distance distributions we extracted the nearest neighbor interaction energy between the pentagons, which exhibit a strong preference to occur in twins, as well as the strain relaxation energy along the pentagon-twin chains.

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## 1. Introduction

The low-index surfaces of the group IV semiconductors have been studied in great detail, except the (110) surface [1–14]. This is quite remarkable given the fact that the (110) is intrinsically anisotropic, in contrast to its (100) and (111) counterparts. The surface free energy per unit area of the (110) surface is higher than that of the (100) and (111) surfaces and therefore the (110) surface has the tendency to facet. The bulk truncated Ge(110) surface has a rectangular symmetry and is composed of zigzag rows of atoms that run in the $[1\bar{1}0]$ direction. The Ge(110) surface reconstructs into rather large unit cells, which are very complex and involve several atomic layers. The most common surface reconstructions of Ge(110) are the ($16 \times 2$) and c($8 \times 10$) reconstructions. Despite a number of detailed studies there is no full consensus yet on the exact model for these reconstructions [1–12]. The ($16 \times 2$) and c($8 \times 10$) are both composed of five-membered atom rings, hereafter referred as pentagons and feature small (17 15 1) facets at the steps. In the remainder of our paper we will adapt the structural models that have been put forward by Ichikawa [8,9]. These structural models of the ($16 \times 2$) and c($8 \times 10$) are consistent with existing scanning tunneling microscopy data. A careful reflection high energy electron diffraction study by Ichikawa, Fujii and Sugimoto [13] revealed that prolonged annealing at temperatures below 650 K resulted in a ($16 \times 2$) reconstructed surface. Therefore we can safely conclude that the ($16 \times 2$) reconstruction is the thermodynamically most stable reconstruction,

whereas the c($8 \times 10$) reconstruction is only a metastable and transient reconstruction. The ($16 \times 2$) reconstruction undergoes an order–disorder transition at temperature of about 700 K. For a detailed description and discussion of the ($16 \times 2$) and c($8 \times 10$) reconstructions, as well as a brief overview of the history of the Ge(110) surface we refer to Ichikawa's papers [2,3,8–10,13] as well as a recent paper by Mullet and Chiang [14]. The vast majority of papers published on Ge(110) deal with the structural properties of the surface, whereas the electronic properties received much less attention [15–17]. Here we present a combined scanning tunneling microscopy and spectroscopy study of the elementary building block, i.e. a pentagon, of the Ge(110) surface. The local density of states of the two most common reconstructions of the Ge(110) surface, i.e. the ($16 \times 2$) and c($8 \times 10$) reconstructions, will be extracted from spatially resolved scanning tunneling spectra. The energetic interaction between the pentagons and the long-range strain relaxation within in the zigzag pentagon rows will be extracted from a statistical analysis of the roughness of the $[1\bar{1}2]$ oriented steps and the kink–kink length distribution within the steps, respectively.

## 2. Experimental

The scanning tunneling microscopy (STM) and spectroscopy (STS) measurements were performed at room temperature in an ultra-high vacuum system with a base pressure of $3.10^{-11}$ mbar. The Ge(110) samples were cut from nominal flat, single-side polished nearly intrinsic (50–60 $\Omega$cm) n-type wafers. After cutting, the samples were thoroughly cleaned with isopropanol alcohol before inserting them into the ultra-high vacuum system. Firstly, the Ge(110) samples were outgassed for

at least 12 h at a temperature of 750–800 K. Secondly, we cleaned the samples by a method that we applied to and tested extensively on the closely related Ge(001) surface [18]. This cleaning method involves several cycles of Argon ion bombardment followed by annealing at temperatures of 1100 ($\pm$25) K. After five to seven of these cleaning cycles the Ge(110) samples were atomically clean and exhibited well-ordered reconstructed (16 × 2) and c(8 × 10) domains as well as some disordered regions. The relative occupation of the various reconstructions can be tuned by varying the cooling time after a high temperature anneal. A slow cooling rate leads to an increase of the (16 × 2) domains at the expense of the c(8 × 10) and disordered domains. Since we aim at a detailed study of all domains we have rapidly cooled down our samples.

## 3. Results and discussion

In Fig. 1A a large-scale filled-state STM image of a Ge(110) surface is shown. The Ge(110) surface exhibits regions with c(8 × 10) and (16 × 2) reconstructions, as well as some disordered regions. In the top right quadrant of Fig. 1A a few (8 × 2) domains can be seen. These (8 × 2) have been reported earlier in Ref. [14]. In the insets of Fig. 1 zoom-ins of the different phases are displayed. Interestingly, all phases, including the disordered phase, are composed of five-membered atom rings (hereafter referred as pentagons). In Fig. 2A and B simplified structural models of the (16 × 2) and c(8 × 10) reconstructions are shown. For the fully relaxed models we refer to the work of Ichikawa [8,9]. In these papers fully relaxed models of the (16 × 2) and the c(8 × 10) reconstructions are shown that are consistent with existing STM data. We would like to emphasize that the (16 × 2) reconstruction, in contrast to the c(8 × 10) reconstruction, consists of alternating up and down row of pentagons (see Figs. 2 and 1C–D). The zigzag rows of pentagons in the c(8 × 10) domains are aligned along the [$2\bar{2}5$] direction, whilst the zigzag rows of pentagons in the (16 × 2) domains are aligned along the [$1\bar{1}2$] direction. Both straight and rough step edges are found on the surface. The straight steps are aligned along the zigzag pentagon rows of the (16 × 2) domains, i.e. along the [$1\bar{1}2$] direction. Both zigzag rows seem to be composed of pentagon twins, however a more careful

inspection of the models (see refs. [8,9]) reveals that the pentagon twins are not exactly the same. For the remainder of this work we will focus our attention on the pentagon twins of the most stable reconstruction, i.e. the (16 × 2) reconstruction.

In Fig. 3A the *IV* spectrum of the bare Ge(110) surface is depicted. The *IV* curves recorded on the different regions of the Ge(110) surface, i.e. the (16 × 2), c(8 × 10) and disordered domains, are essentially the same. This is not so strange since all reconstructions/phases are composed of the same elementary building blocks, i.e. the pentagons. In addition, *IV* curves recorded on the pentagons of the different regions (domains) do not reveal any detectable differences.

In Fig. 3B and C the differential conductivity (*dI/dV*) and the normalized differential conductivity (($dI/dV)/(I/V)$) are shown. All *IV* traces are recorded with the same set points of V = −1.5 V and I = 0.25 nA. In Fig. 3D an STM image recorded at the used set points is depicted. In the normalized differential conductivity spectrum three well-defined peaks are resolved: two filled-states at −1.1 V and −0.3 V respectively and an empty-state at 0.4 V. In Fig. 3E and F STM images recorded at 0.4 V and −0.35 V are shown. In contrast to Fig. 3D, where a clear structure in between the zigzag pentagon rows appears, Fig. 3E and F are composed of pentagons only. Since to the best of our knowledge no spectroscopic data of the Ge(110) is available, we compare our results with spectroscopic data recorded on the closely related Si(110) − (16 × 2) surface [19–21]. Setvín et al. [19] performed a very detailed study on the electronic structure of the Si(110) surface. In contrast to the Ge(110) surface, Setvín et al. found at least three electronic states for the Si(110) surface. Two electronic states are located very close to the Fermi level, one about 0.2 eV below the Fermi level and about 0.2 eV above the Fermi level. These two states near the Fermi level can be ascribed to the pentagons, which are also the elementary building block of the Si(110) − (16 × 2) surface. Another filled state at −1.5 V is located in the middle of the pentagons and was ascribed to the underlying zigzag line of Si atoms. The energy of this electronic state is high enough to be assigned to Si−Si back bonds. The electronic states we have found for Ge(110) at −0.3 V and 0.4 V are both related to the pentagons, but our room temperature STS data has insufficient spatial resolution to resolve the exact position of the electronic states within the pentagons. The electronic state of Ge(110) located at −1.1 V is also clearly present
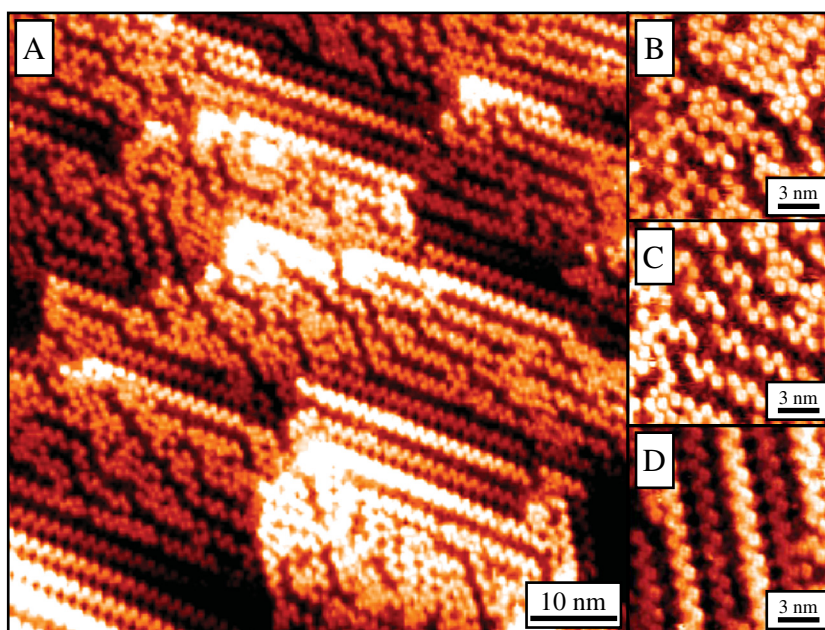


**Fig. 1.** (A) Filled-state scanning tunneling microscopy image of Ge(110). (B) Scanning tunneling microscope image of the disordered phase. (C) Scanning tunneling microscope image showing a region that exhibits a c(8 × 10) phase (middle part of the image) as well as a disordered phase (at the left and right border of the image). (D) Scanning tunneling microscope image of the (16 × 2) phase. Set points are (A) −1.5 V, 0.5 nA, (B) −1.5 V, 0.29 nA, (C) −1.5 V, 0.29 nA and (D) −1.5 V and 0.29 nA.