

INVESTIGATION OF THE VICINAL Ge(001) SURFACE WITH STM

BART A.G. KERSTEN, LIANDA SJERPS-KOOMEN, HAROLD J.W. ZANDVLIET,
AND DAVE H.A. BLANK
University of Twente, Department of Applied Physics, P.O. Box 217, 7500 AE Enschede,
The Netherlands

ABSTRACT

The morphology of Ge(001) has been investigated with a UHV - Scanning Tunneling Microscope. The Ge(001) surface was misoriented towards the [011] direction with a miscut angle varying from 0.4° to 5°. The surface stress was found to have considerable influence on the step edge configuration as well as the position of the steps with respect to each other.

INTRODUCTION

Recently there is increased interest in the morphology of vicinal crystal surfaces i.e. surfaces slightly misoriented with respect to a low index direction. The misorientation is typically accommodated by single or double height steps which separate terraces of the low index direction. This interest rises from the important role steps play in phenomena as crystal growth chemistry, catalysis and the growth of epitaxial overlayers.[1-3] Most attention has been focused on the Si(001) surface with a small miscut θ towards the [011] direction.

Both, the Ge(001) and the Si(001), surface reconstruct by forming dimers that are arranged in parallel rows. Depending on the plane where the crystal is cut either a (2 x 1) or (1 x 2) reconstructed domain is formed, which are related to each other by a 90° rotation. If the surface has a slight miscut θ towards the [011] direction, single height steps are formed, which separate terraces with alternatingly a (2 x 1) and (1 x 2) reconstruction. In this configuration two types of steps denoted SA and SB occur.

For Si(001) it is observed that with increasing θ the SB step shifts towards the lower lying SA step [4,5]. For θ greater than 2° this leads to the formation of double height DB steps and for $\theta > 4^\circ$ the SL steps have almost disappeared and a primitive (2 x 1) surface is formed. Here we present and discuss the transition we have measured for Ge(001), from SL to SB steps and show that its behaviour is in some extent similar to silicon. The transition from SL to DB steps is especially influenced by surface strain [4-7]. In this paper we will show that the surface strain also has a large impact on the configuration of steps. We have observed a type of SB steps that has not been reported before and will present a configuration that incorporates strain effects.

EXPERIMENTAL

All experiments were carried out in a stainless steel ultra high vacuum chamber with a base pressure of 1.10^{-10} Torr. The chamber contains an Omicron UHV STM, a CMA Auger apparatus, an ion gun as well as facilities for gas handling. The 5 x 10 mm Ge(001) substrates

were miscut towards the [110] direction by 0.4, 1°, 2°, 3° and 5° respectively.

Before loading in the UHV system they were ultrasonically rinsed in isopropyl alcohol. No further chemical treatments were used. The sample could be heated resistively by passage of a DC current. A clean surface was obtained by cycles of sputtering (1000 eV, Ar ions $2\mu\text{A}/\text{m}^2$ 30 min., angle of incidence 20°) and annealing ($800\pm 50\text{K}$, 20 min.). The temperature during annealing was measured with an infrared pyrometer. After annealing the samples were radiation quenched to room temperature by disconnecting the heating current. STM images were taken in the constant current mode with a sample bias between -1 and -2V and a typical tunnelling current of 5 nA. Scan ranges varied between $700 \times 700\text{\AA}$ and $1000 \times 1000\text{\AA}$ (0,8 to 1,0 $\text{\AA}/\text{pixel}$). The scanning direction was oriented 45° to the dimer rows.

To get reasonable statistics several images were taken to achieve a total length of the SB step greater than $3600 a$ (a is raster constant) for each miscut angle.

RESULTS AND DISCUSSION

An interesting feature of the Ge surface is that the SB steps are much rougher i.e. have more thermally excited kinks than the SA steps (see fig. 1.) which is consistent with measurements on Si(001) [7-9] Analysis of the kink distributions have been used to determine step- and interaction-energies.

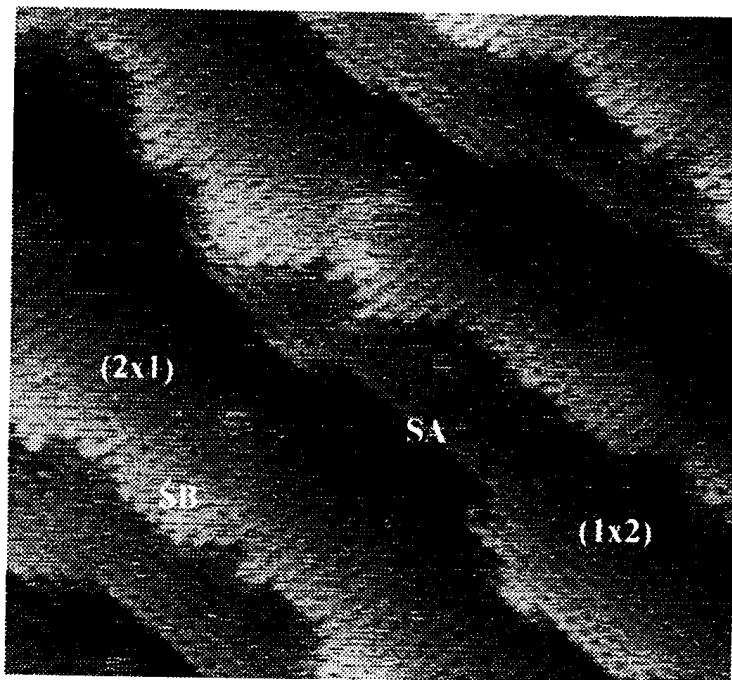


Fig. 1 STM measurements of Ge(001) misoriented towards the [001] direction by 1°. SA steps and (1 x 2) terraces alternate with SB steps and (2 x 1) terraces. Scan range is $400 \times 400\text{\AA}$. $I = 3.5\text{ nA}$, $V = -0.5\text{ V}$.

In contradiction with Si(001) the Ge(001) surface exhibits two kinds of SB steps. In principle there are two different geometries for the SB step depending on the way the SB step ends with respect to the lower lying terrace (see fig. 2). The SB step can be rebonded or non-bonded, the latter configuration being rare on Si(001) [7-11]. Chadi [10] performed calculations on Si(001) steps which showed the rebonded SB step to be more stable than the non-bonded.

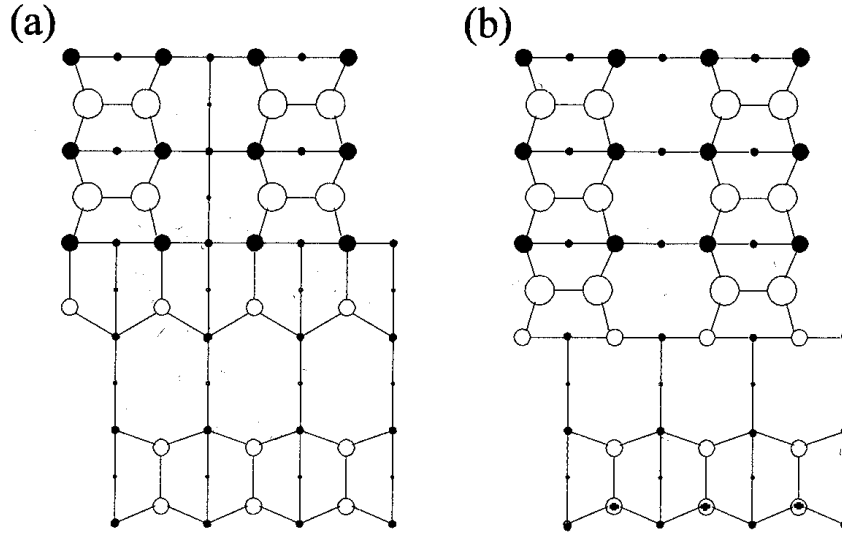


Fig. 2. (a) - (b) Top views of the rebonded (a) and the non-bonded (b) SB step, respectively, after ref. [10]. Larger circles denote atoms with a dangling bond. A crossing is used to indicate buckling away from the substrate.

The energy difference between them is roughly equal to the energy difference between the rebonded SB and SA step (0,16 eV/a). For the lowest miscut angle the effect of strain is the smallest, resulting in an equal population of the rebonded and non-bonded SB steps. This indicates that for germanium the energy difference is much smaller than for silicon.

To understand the morphology of steps, the surface stress must be taken into account. The dimer bond induces considerable stress, a tensile stress in the direction of the dimer bond and a compressive one in the perpendicular direction, i.e., a single domain say (2 x 1) surface can lower its energy by contraction in the direction of the dimer bond and expansion in the direction along the dimer rows [12]. This anisotropy in surface stress is partly responsible for the energy difference between the rebonded and the non-bonded SB step. The rebonded SB step has stretched bonds at the step edge, which can be stabilised by a relaxation of the dimer row in the direction along the dimer row.

Our measurements show two clear examples of the influence of the anisotropy of the surface stress. First, consider in fig. 2b the dimer at the edge of the SB step. The two dimers that lie in front of it on the lower (1 x 2) terrace show the same kind of buckling in all our measurements. The two dimers are buckled in the same direction and the buckling is such that the dimers closest to the SB step are the lower ones. This buckling can be explained by the tendency of the (2 x 1) dimer row to expand itself, which tends to shift the atoms on the lower (1 x 2) terrace away from the step edge. Second we have found a deviant configuration for the non-bonded SB step which has not been reported so far. In figs. 3a,b this

configuration can clearly be seen. This configuration occurs together with the normal configuration of the non-bonded SB step of fig. 2b: the ratio being about 1 to 1. It was observed for all miscut angles in all measurements and is characterised by a single dimer that ends two dimer rows of the (2 x 1) terrace.

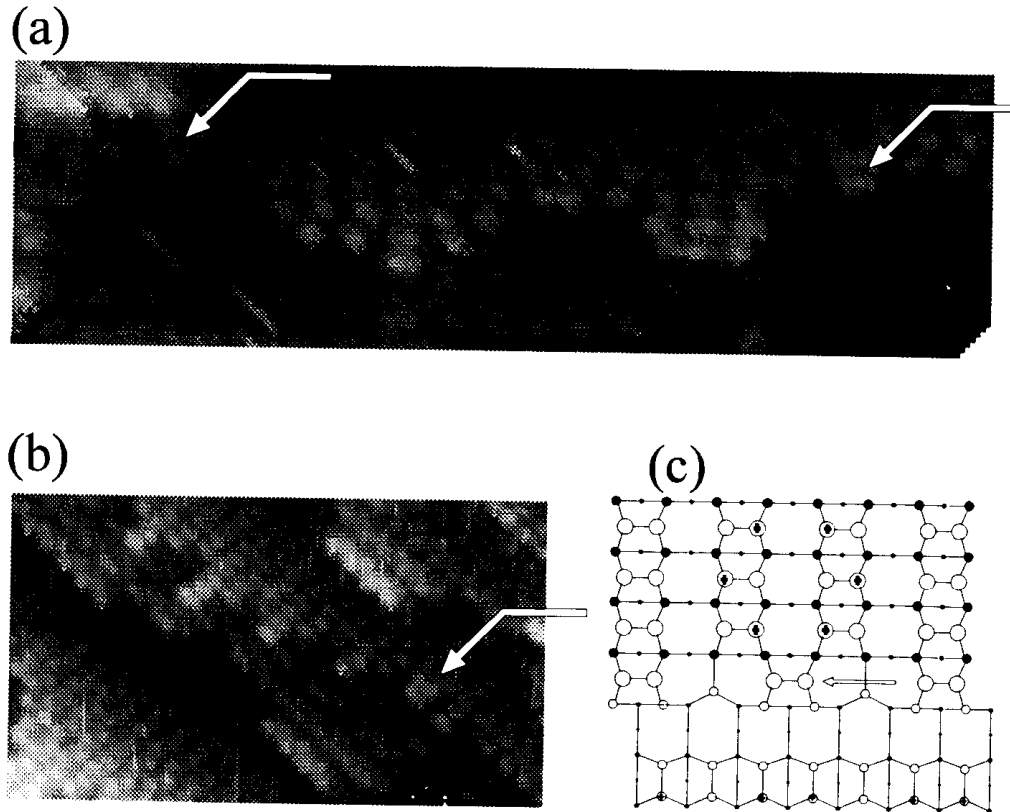


Fig. 3 (a) - (b) Close-ups of a 30° misoriented surface, $I = 5 \text{ nA}$, $V = -2 \text{ V}$. Scan range is about $80 \times 30 \text{ \AA}$ for (a) and $100 \times 50 \text{ \AA}$ for (b). Both rebonded, non-rebonded, and deviant-non-bonded SB steps occur. The arrows point to the "end dimer". Note the buckling of the (1 x 2) terrace dimers in front of the non-bonded SB edge-dimer.

(c) Proposed configuration for the non-bonded SB step. Open circles denote atoms with dangling bonds, larger circles denote atoms of the upper terrace, a cross indicates buckling upwards from the substrate. The arrow points to the "end dimer". The atoms next to the end-dimer are rebonded.

We have two arguments that this "end dimer" is a dimer and not an effect caused by two buckled dimers. First, height differences at both sides of the end dimer are 1,0 Å. Height differences caused by buckling are rarely higher than 0,5 Å. Second, as mentioned above, the dimer at the edge of a non-bonded SB step is always accompanied by the same kind of buckling at the lower (1 x 2) terrace. In the measurement of fig. 3a,b only the dimers of the (1 x 2) terrace in front of the "end dimer" have this buckling. The configuration is a mixture of a rebonded and non-bonded SB step and has a periodicity of 3a along the step edge.

Table 1

θ	p	% DB	% rebonded SB
1	0.249	2.0	51.0
2	0.388	4.1	52.2
3	0.338	11.2	59.6
5	0.305	37.7	80.3

With increasing θ we observe an increase of the percentage of rebonded SB step over the non-bonded one (see Table 1). Further, the percentage of DB steps increases and a shift of the SB step towards the lower lying SA terrace is observed. Let 2ℓ be the average distance between the SA steps and $(1+p)\ell$ the size of the (2 x 1) terrace, so p describes the asymmetry between the 2 x 1 and the 1 x 2 terrace sizes. In Table 1 the percentage of double steps DB and p are presented as function of θ . These measurements show roughly the same behaviour as those for silicon. From measurements on silicon a theoretical framework has been developed [5,6,13-15] that takes into account step energies and surface stress. The influence of surface stress has been described in terms of monopole-monopole and dipole-monopole interactions. Following Phelke and Tersoff [6] the energy of a SB + SA pair is :

$$E = \lambda_0(SA + SB) - 2\lambda_\sigma \cdot \ln\left(\frac{\ell}{\pi a} \cos\left(\frac{p\pi}{2}\right)\right) + \lambda_d \left(\frac{a}{2\ell}\right)^2 - (3\lambda_\sigma \cdot \lambda_d)^{1/2} \frac{a}{\ell} \tan\left(\frac{p\pi}{2}\right)$$

The first term is the step energy of the SA and SB step excluding strain contribution to the energy. The second term is the Alerhand's energy and describes the force-monopole-monopole interaction. The third and fourth term describe the monopole-dipole interaction.

Calculations [10] for silicon show that $\lambda(DB) < \lambda(SA) + (SB)$. In the case of Ge(001) only for $\theta = 5^\circ$ a sharp increase of the percentage of DB steps is observed. This contradiction can be explained by the Alerhand's [13] energy and the rebonding of the SB steps. The first states that the strain energy of a surface with alternatingly (1 x 2) and (2 x 1) domains is lower than the strain energy of a single domain surface consisting exclusively of DB step. The rebonding of the SB steps induces a dipole-monopole interaction and a lowering of the strain energy by a shift of the SB terrace towards the lower lying SA terrace [5,6]. This accounts for the increase of p in Table 1 for small θ , but also for the increase of the percentage of rebonded SB steps we observe. The dipole-monopole interaction becomes stronger with decreasing terrace width.

The force dipole is ascribed to the rebonding of the SB step. For the non-bonded or partly bonded configuration we have proposed, the force dipole may assumed to be lower. Hence with increasing θ the rebonded SB step will be energetically more favourable than the non-

bonded. The decrease of p for $\theta > 3^\circ$ is caused to by the relatively small terrace width ; kinks of length $2a$ already have a large impact on p .

In conclusion, we have found that the surface stress is an important factor in the morphology of the vicinal Ge (001) surface. It influences the configuration of the step-edges, as well as the position of the steps with respect to each other.

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