D_A Steps and 2D Islands of Double Layer Height in the SiGe(001) System

Matthias Kummer, Bernhard Vögeli,* Thomas Meyer, and Hans von Känel

Laboratorium für Festkörperphysik, ETH Zürich, CH-8093 Zürich, Switzerland

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The surfaces of step graded, partially relaxed $Si_{1-x}Ge_x/Si(001)$ buffers were studied by scanning tunneling microscopy. The surface slips along $\langle 110 \rangle$ forming the crosshatch pattern, consisting of bunches of D_A steps of double layer height. The D_A steps are present in regions of large surface gradients close to the slips, as well as in planar regions between the slips. These regions are also characterized by the appearance of 2D islands of double layer height. The observations can be explained by assuming the strain due to the misfit dislocations to be locally anisotropic. Anisotropic misfit strain and efficient strain relaxation by the (2×8) Ge reconstruction were identified as the main factors causing the unusual step structure.

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The step structure of the Si(001) surface has been attracting much attention in the past two decades due to the unrivaled importance of Si as an electronic material. Exact knowledge of the initial step structure and its evolution is indispensible in order to understand epitaxial growth.

The surface steps on singular or slightly misoriented clean Si(001) are of monolayer (ML) height. The Si(001) surface exhibits a characteristic (2×1) reconstruction with dimer rows oriented perpendicular to one another on adjacent terraces. The terraces are bounded by two distinct types of steps: S_A steps to which the upper-terrace dimer rows are oriented parallel, and S_B steps to which they are perpendicular. By contrast, steps of double layer height are not stable on these surfaces. Bilayer D_B steps, with dimer rows perpendicular to the step edge, can be stabilized by applying uniaxial stress [1]. D_B steps also become stable on vicinal surfaces for misorientation angles above 2.5° [2]. By contrast, D_A steps have never been observed on clean Si surfaces, because their energy is much too high [3,4].

The behavior is different when Ge or $Si_{1-x}Ge_x$ alloys are grown epitaxially on vicinal or uniaxially strained Si surfaces. In both cases the high-energy D_A steps have been found to form [5,6]. For vicinal surfaces strain relaxation by dimer vacancy lines (VLs) is thought to be responsible for the preference of D_A steps [6]. For Ge-rich alloys on well-oriented but uniaxially strained Si substrates the surface stress field favors the domain for which the dimer lines are along the direction of the applied compressive stress, leading to the same result [5].

In this Letter, a third configuration leading to D_A steps will be discussed, i.e., partially relaxed step graded $Si_{1-x}Ge_x$ buffers on Si(001). Step graded SiGe buffer layers serve as virtual substrates for novel devices, such as the Si modulation doped field-effect transistor, requiring a strained Si quantum well in order to exhibit high electron mobility. Ultimate device performance may depend critically on the step structure at the epitaxial interfaces. Exact knowledge of the *surface* step structure on graded buffer layers may therefore be of practical importance.

The films were grown on well-oriented Si(001) substrates by rf magnetron sputter epitaxy. Details of the sputter system, the sample preparation, and the growth conditions are described elsewhere [7,8]. A 1000 Å Si buffer, grown at 500 °C, separated the substrate from the step graded buffer, which was grown at 485 °C. Starting with a Ge mole fraction of $x = 0.12$, x was raised in increments of $\delta x = 0.01$, up to the final Ge mole fraction of $x_f = 0.30$. Typical growth rates were between 1.5 (pure Si) and 2.1 Å/s for $Si_{0.7}Ge_{0.3}$. The total thickness of the graded buffer was 500 nm, which results only in a partial relaxation of the misfit strain.

The surface of step graded $Si_{1-x}Ge_x/Si(001)$ buffers exhibits a so-called crosshatch pattern, which is formed by surface slips associated with the pileup of misfit dislocations (MDs) running along the $\langle 110 \rangle$ directions [9]. As will be shown in the following, the local strain associated with this crosshatch pattern affects the surface step structure decisively.

Figure 1 shows a scanning tunneling microscopy (STM) image of the step structure in the region of a surface slip. Because of Ge segregation, the surface is (2×8) reconstructed, the larger period of the reconstruction being formed by lines of dimer vacancies oriented perpendicular to the dimer rows [10]. All dimer VLs are aligned perpendicular to the surface slip, the latter being formed exclusively by D_A steps of double layer height. The sole presence of double layer steps follows immediately from the fact that all VLs have the same orientation in Fig. 1. It is important to emphasize that STM images taken in many different surface areas show that the occurrence of D_A steps does not require the surface gradient to be large. By contrast, D_A steps are present also in more planar regions, such as the one shown in Fig. 2. The inset shows the structure resolved in more detail, and emphasizes that the VLs are aligned across the surface steps.

Let us first discuss the occurrence of D_A steps close to a surface slip, as shown in Fig. 1. On counting the number of steps present in the region of the surface slip ($\approx 8D_A$), we may conclude that the slip must be the signature of a

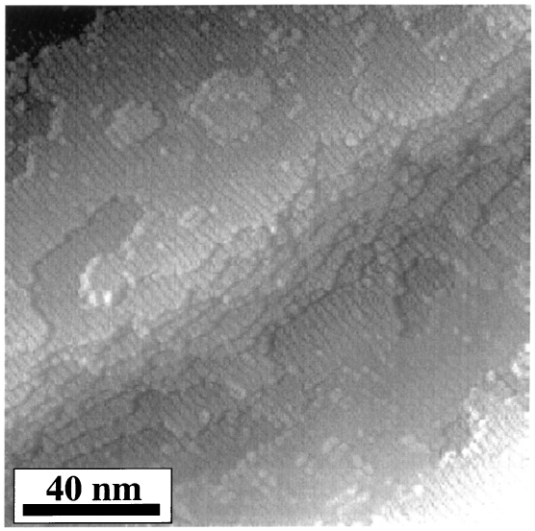

FIG. 1. The step structure of a relaxed, graded $Si_{0.70}Ge_{0.30}$/Si(001) buffer. The high local misorientation at the surface slip favors D_A steps of double layer height, with the dimer vacancy lines (VLs) perpendicular to the steps.

pileup containing several dislocations. This may be seen as follows: One single misfit dislocation with Burgers vector $\vec{b} = a/2\langle 011\rangle$ leads to a surface slip of $a/2$ where a is the Si lattice parameter. Hence the slip of $8D_A$ observed in Fig. 1 must be due to $\approx$8 dislocations present on closely spaced $\langle 111\rangle$ planes. The (2×8) reconstructed terraces in the region of the step bunch are very narrow ($\approx$50 Å on average), a situation closely resembling the one of a pseudomorphic $Si_{1-x}Ge_x$ alloy grown on a Si(001) substrate misoriented by 3.1°. Thin $Si_{1-x}Ge_x$ layers on such *vicinal* Si(001) surfaces were shown to exhibit D_A steps [6], as a result of the efficient strain relaxation by the (2×8) reconstruction when the dimer VLs are oriented perpendicular to the steps [10].

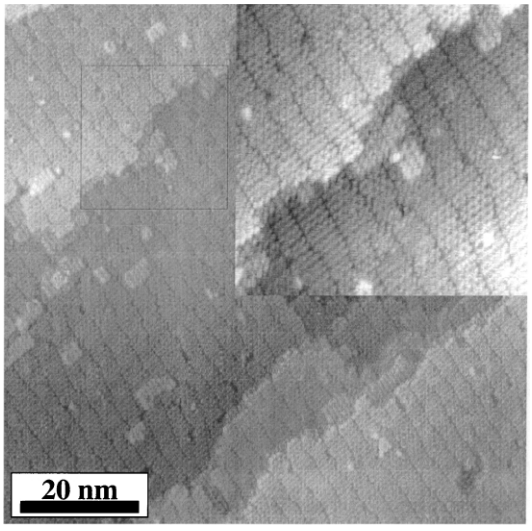

FIG. 2. D_A steps form even in planar regions, despite their higher energy per ledge atom. The inset shows that due to the short-range attractive interaction between single dimer vacancies on adjacent dimer rows, the VLs are aligned across a step of double layer height.

On flat surfaces, i.e., for larger terraces such as the ones present in Fig. 2, the argument no longer holds, and we might expect the step structure to revert to monolayer steps. Yet Fig. 2 shows the exclusive presence of D_A steps even in these regions. Similar observations have been made in other quasiplanar regions in the vicinity of a small surface slip, and in the regions farther away from the ridge sidewalls of larger slips, such as the one of Fig. 1. Note also that according to the inset of Fig. 2 the VLs are aligned across the D_A steps. This indicates that the (2×8) reconstruction influences the step structure decisively even in these quasiplanar regions. The occurrence of the (2×8) reconstruction as such does not, however, explain the observed step structure, since it is also present on biaxially strained alloy surfaces, and these exhibit exclusively monolayer S_A and S_B steps. There must hence be an additional mechanism at work here, which we can identify with *anisotropic strain* as follows: The MDs release misfit strain locally in the direction perpendicular to the slip. As a result, the misfit stress becomes anisotropic in this region, with the direction of higher compressive stress parallel to the MDs.

Generally, the (2×8) reconstruction releases more misfit strain perpendicular to the VLs than parallel to them [10]. Thus, if anisotropic strain is present, it is favorable to align the VLs perpendicular to the direction of larger compressive strain. We may hence conclude that the anisotropic strain in the vicinity of a surface slip will favor the alignment of the VLs in the direction perpendicular to the slip. This obviously requires adjacent terraces to be bounded by D_A steps and hence explains our observations presented in Fig. 2. Our STM studies on buffer layers which are close to the onset of strain relaxation (not shown) indicate that the transition from monolayer steps to D_A steps takes place even when very few MDs are present. This emphasizes the sensitivity of the step structure on local stress anisotropies.

A close inspection of the STM images reveals that the bilayer steps are present not only at the boundary of large terraces. The 2D islands present in the planar regions and marked by the arrows in Fig. 3 are all of double layer height as well. This follows immediately from the fact that the VLs on these islands are oriented parallel to those in the adjacent surface regions. By contrast, 2D islands of double layer height never form on *unstrained* Si(001) and Ge(001) surfaces. Similarly, 2D islands on *biaxially* strained $Si_{1-x}Ge_x$/Si(001) layers remain of monolayer height. The presence of the 2D islands of double layer height must hence again be related to the locally *anisotropic* strain due to the crosshatch pattern [11], and to the way in which this strain affects the (2×8) reconstruction, as will be discussed in more detail below.

In order to get a more quantitative measure of the strain anisotropy, this quantity was evaluated directly from the STM images in the following way.

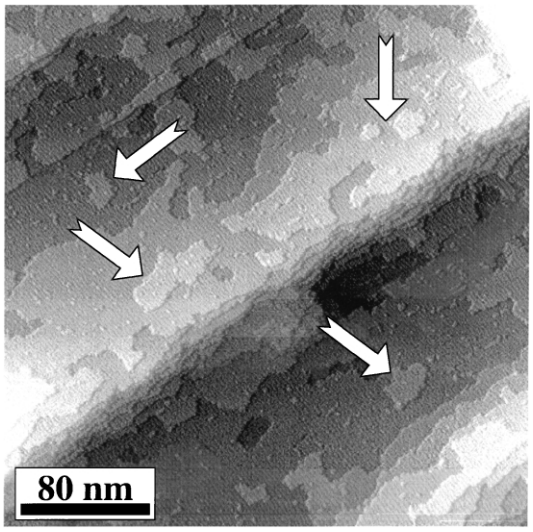

FIG. 3. The islands marked by the arrows are of double layer height, as can be concluded by comparing the orientation of the VLs on the islands and the surface underneath. Figure 1 shows the upper right quarter of this figure in greater detail.

From STM cross sections taken in the direction perpendicular to a slip line the surface deformation was obtained as a function of the distance from the slip. These profiles were then fitted to the theoretical expressions describing the surface distortion caused by the strain field around buried misfit dislocations. The number of dislocations giving rise to the slip in question followed directly from the slip height. For strain modeling elastic isotropy was assumed. The displacement field was calculated for a free surface by applying the method of image dislocations [12] to the edge component of dislocations with Burgers vector $\vec{b} = \frac{a}{2}\langle 011\rangle$, under the additional constraint of zero net force in the direction perpendicular to the surface. For the fits of the calculated surface displacements to the measured STM profiles, the dislocations were allowed to be arbitrarily distributed between the interface and a shallowest depth L, with L entering as a fit parameter. A value of L consistent with cross-section transmission electron microscopy of 200 nm was found to give very good fits. Finally, the component ε_{xx} of the strain tensor in the direction perpendicular to a given slip was obtained from the derivative of the appropriate displacements and the misfit stress. Since great care was excercised in order to insure that any perpendicular slip lines were far from the analyzed region, the strain component parallel to the slip, ε_{yy}, is given directly by the misfit stress. The strain anisotropy is then defined as $\delta = |\varepsilon_{xx} - \varepsilon_{yy}|/|\varepsilon_{xx} + \varepsilon_{yy}|$.

Since the formation of the 2D islands of double layer height is connected with the (2×8) reconstruction, there must be a critical lateral size beyond which a transition from monolayer height to bilayer height occurs. More precisely, we expect an island's extension, N, in the direction perpendicular to the VLs of the surrounding region to determine whether it is energetically favorable to grow to double layer height, since in this direction the (2×8) reconstruction will be most effective in releaving the anisotropic misfit strain. In this scenario, cf. Fig. 4, islands of monolayer height would nucleate, grow laterally at first, and then double in height after reaching a critical size, N_c, the latter depending on the local strain anisotropy.

For a statistical analysis of island height versus island size, more than 60 islands located in five regions of two identical STM samples were analyzed. The islands could be assigned to three groups, with strain anisotropies of $\delta = (4.0 \pm 0.6) \times 10^{-3}$, $(2.8 \pm 0.4) \times 10^{-3}$, and $(1.6 \pm 0.3) \times 10^{-3}$, respectively. Figure 5(a) shows the second layer coverage of the islands versus their lateral extension, N, in units of VLs. This plot suggests that both the critical lateral size, N_c, and the range of ΔN within which the transition takes place, depend on the local strain anisotropy. The larger the strain anisotropy the smaller N_c and ΔN, giving rise to a curve with a lower onset saturating very quickly. With decreasing anisotropy saturation to double layer height becomes more and more gradual, until for biaxially strained regions the islands are of monolayer height for all N.

In order to describe the data of Fig. 5 in terms of a thermodynamic model, the energies of the relevant steps ought to be balanced in the presence of anisotropic strain. These numbers are not available, however, and their *ab initio* calculation is beyond the scope of this Letter. On the other hand, the data can equally well be described by a phenomenological kinetic model in which the effect of the strain anisotropy on the island height is cast into an asymmetric Schwoebel barrier [13]. This barrier is assumed to be operative at the bounding step of an island of monolayer height. The probability for an adatom to cross the step in the up direction and in the down direction is designated as P_{up} and P_{down}, respectively. The ratio $P_{\text{up}}/P_{\text{down}}$ is assumed to be given by the local strain anisotropy at the position of the island, δ, and by the size of the island area

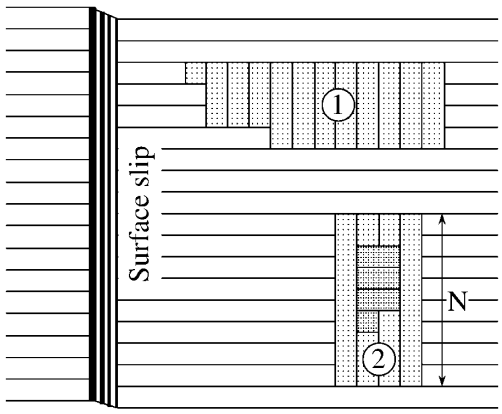

FIG. 4. When the lateral extension of an island in the direction perpendicular to the VLs underneath, N, exceeds a critical value, N_c, the second layer starts to form. Despite the larger area of island 1, N_c is exceeded only for island 2. The black lines represent the VLs, running perpendicular to the slip line indicated on the left-hand side.

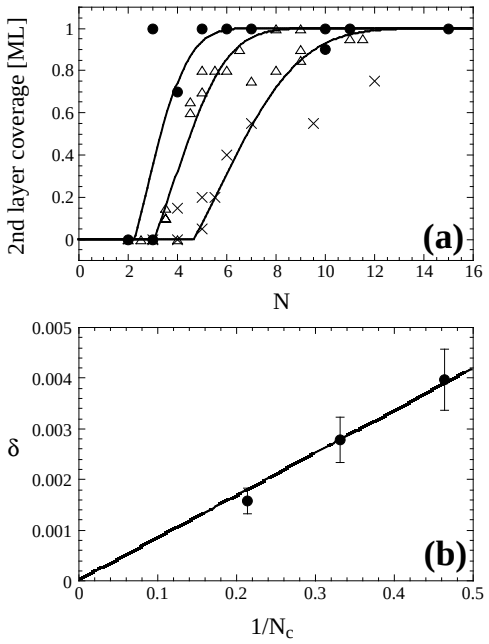

FIG. 5. (a) The second layer coverage of a 1 ML high island as a function of its lateral extent N in units of VLs for islands found in regions with high (•), intermediate (△), and low (×) strain anisotropy, determined from the STM images as $\delta = (4.0 \pm 0.6) \times 10^{-3}$, $(2.8 \pm 0.4) \times 10^{-3}$, and $(1.6 \pm 0.3) \times 10^{-3}$, respectively. The solid lines result from a fit to a model assuming an asymmetric Schwoebel barrier due to strain anisotropy. (b) The reciprocal of the critical island size, $1/N_c$, is plotted against the experimentally determined strain anisotropy, δ.

remaining at monolayer height. Considering for simplicity circular islands with radius r, the barrier asymmetry is hence taken to be $P_{\text{up}}/P_{\text{down}} = 1 + \alpha\delta(r_{\text{ML}} - r_{\text{DL}})$. Here, r_{ML} is the outer radius of the island, r_{DL} is the radius of the second layer part, assumed to be circular in shape as well, and α is a constant.

The asymmetric Schwoebel barrier causes the adatom concentration to be higher on top of the monolayer island, leading to the nucleation of a second layer growing rapidly at first, and then slowing down as the entire island approaches double layer height. According to the model, δ is predicted to be proportional to $1/N_c$. In Fig. 5(b) the fitted values of $1/N_c$ are plotted against the strain anisotropy δ evaluated *experimentally* from the STM images in the way described above. The data points do indeed scatter around a straight line through the origin, indicating good agreement between the model and the STM data.

In conclusion, we have observed the surface step structure of partially relaxed, graded $Si_{1-x}Ge_x/Si(001)$ buffers to reveal D_A steps and 2D islands of double layer height. D_A steps are a result of the locally anisotropic misfit strain due to the pileup of misfit dislocations. Anisotropic strain and the possibility of the (2×8) Ge reconstruction to release more strain perpendicular to the VLs lead to 2D islands of double layer height. The nucleation and growth of the second layer are well described by a phenomenological model in which a strain-induced asymmetric Schwoebel barrier is assumed.

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*Present Address: Advanced Research Laboratory, Hitachi Ltd., Hatoyama, Saitama 350-0395, Japan.

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