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Trench Formation in Surfactant Mediated Epitaxial Film Growth of Ge on Si(100)

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Abstract. We have used STM to study the surface morphology of thin epitaxial Ge films grown on Si(001) in the presence of the "surfactant" As. The surfactant forces layer-by-layer growth up to 12 ML Ge coverage which could partly be explained by the geometrical surface arrangement of the growing film. Beyond 12 ML coverage we observed a network of trenches which decorate the earlier described *V*-shaped defects inside the film. Overgrowth of such defects is studied and a mechanism discussed.

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The epitaxial system Ge on Si(001) is known to be of the Stranski-Krastanov (SK) type [1–4]. Up to the critical thickness of 3 ML Ge grows in pseudomorphic layers [1 ML (monolayer) = 6.78×10^{14} atoms/cm^2]. If the coverage is increased, the growth of Ge will run through an intermediate phase, the formation of regular faceted, well ordered islands which are called "hut clusters" due to their shape. Beyond this coverage 3D islands appear.

Recently Copel et al. achieved layer-by-layer growth of Ge on Si(001) by saturating the Si surface dangling bonds with arsenic during growth [5]. By means of medium energy ion scattering (MEIS) it could be shown, that it is possible to achieve layer-by-layer growth of an island and a defect free film up to a coverage of 12 ML. At higher coverages the increasing strain of the growing film is relieved by a sudden breakthrough of so-called "*V*-shaped defects" [6, 7].

This defect can be described as two $\Sigma 9$ grain boundaries in the $[1\bar{1}2]$ and $[1\bar{1}\bar{2}]$ direction [8]. Several $\{111\}$ planes are enclosed which provide strain relief by their smaller layer distance. The *V*-shape of the grain boundaries makes it possible to relieve the strain gradually while increasing the film thickness.

The way the surfactant works is not yet fully understood. Therefore the goal of the investigation presented was to contribute surface sensitive information about the layer morphology during growth.

We used 50 mΩ Si(001) samples with a random miscut of about 0.07°. After degassing the surfaces were cleaned by thermal desorption of the native oxide at 1050° C followed by several short temperature flashes to 1250° C. Germanium was deposited onto these samples from a boron nitride crucible. The evaporation was monitored by a quartz microbalance. The growth took place at a temperature of 490° C and at a rate of about 2 ML/min. Prior to growth the Si surface was passivated by one monolayer of As at 500° C. A pressure of about 8×10^{-8} mbar As in the form of As_4 was supplied during Ge growth using an effusion-cell. These experimental conditions are comparable to the ones used in [5].

Arsenic forms a stable (2 × 1) reconstruction on Si(001) [9–11]. The experimental conditions chosen leave the surface As capped before and after deposition. Therefore, all presented STM micrographs do not show pure semiconductor surfaces but a complete As layer. Since there are only few references for an STM or other detailed topographic work of As on Si(001) ([11] studies Si(001):As surfaces with high step density) we first checked the influence of As on the pure Si(001) surface (see Fig. 1). The surface is well ordered in a nearly perfect (2 × 1)-reconstruction with no missing dimers. Wheras the pure Si(001) surface has a strong tendency towards asymmetric and buckled dimers, the As-(2 × 1) consists of symmetric dimers [10, 11].

The initially atomically flat silicon surface has roughened drastically. The surface is not just homogeneously covered by a layer of arsenic as it is usually assumed for passive capping [5]. All terraces are covered by small islands but still consist mainly of only two levels. The coverage in the third level is very low (< 5%). The appearance of the dimers is the same between and on top of these islands. On the other hand, the maximum As coverage is 1 ML, because there are no dangling bonds left, where excess As could bond to. The

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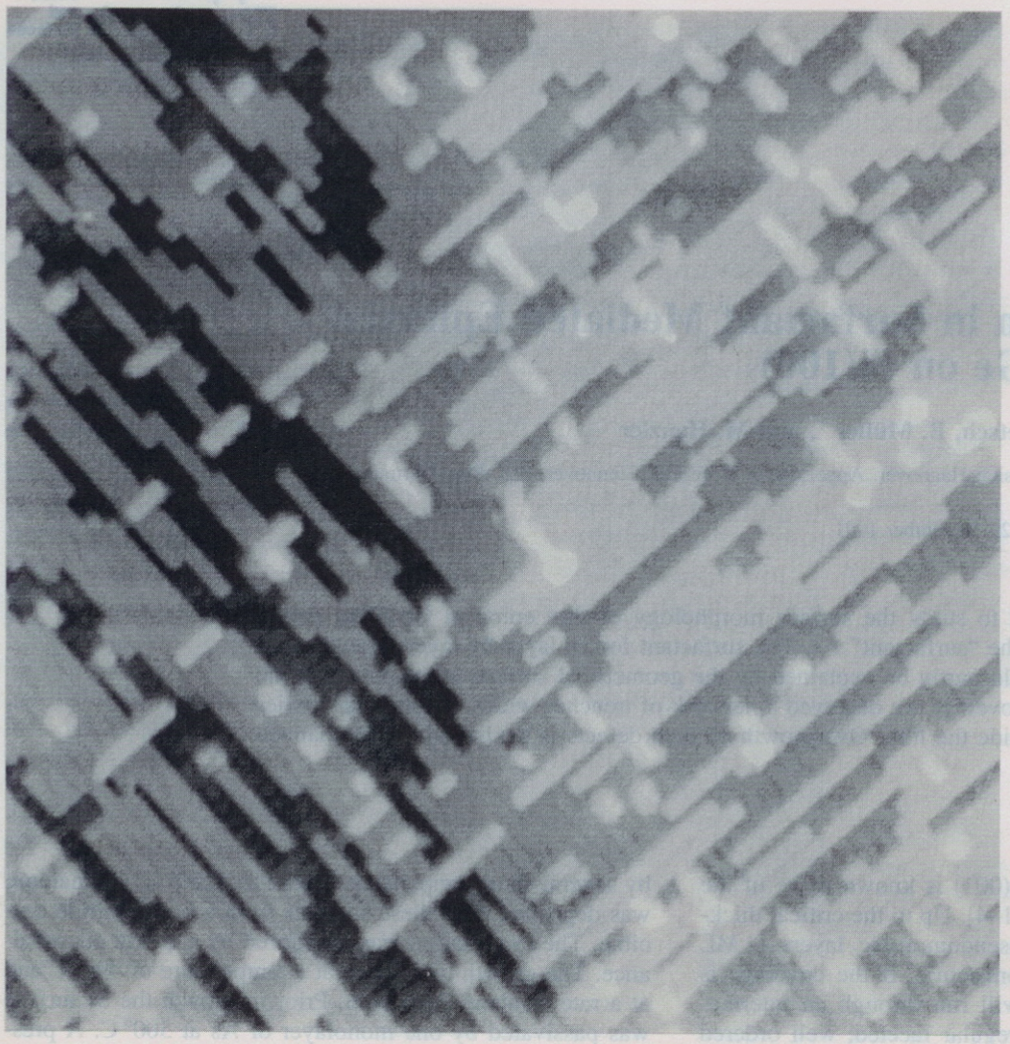

Fig. 1. STM image of an As-(2 × 1) covered Si(001) surface. The roughness is much higher than on a pure Si(001)–(2 × 1) surface influencing nucleation and growth characteristics. (Image size: 450 Å × 450 Å)

only possible conclusion is that 1 ML of arsenic covers the surface completely but the underlying silicon has changed its morphology. A strong tendency to long rows of single dimers is apparent.

Deposition of up to 12 ML Ge on this surface leads to epitaxial non-islanding layer-by-layer growth. Figure 2 was scanned after deposition of about 12 ML Ge. The terraces have very rough edges similar to "fingers" perpendicular to the edge with a length ratio of about 1:5 to 1:8. Ge growth on Si(001) without arsenic coevaporation shows only weakly anisotropic islands [4]. We did not find any "hut clusters" beyond 3 ML coverage. The roughness is only two-dimensional i.e. the vertical height distribution has only two levels per terrace. Additionally we find no hint of any bulk defect in accordance with TEM results.

As already seen on the Si(001):As surface without Ge coverage, the islands are extremely anisotropic. There are only few nucleated islands on top of the finger-shaped large islands. The growth is dominated by step flow according to the high deposition temperature. After increasing the Ge-coverage to 24 ML we observed a network of linear trenches parallel to [110] or [$1\bar{1}0$]. Figure 3 shows an area of about 2500 Å × 1500 Å with a network of trenches separating large islands. Most of these trenches are not filled i.e. they are deeper than our tip could resolve. The inset in Fig. 3 shows a height profile perpendicular through one of the dark lines proving that they are at least 6 Å deep. We identify these trenches as being caused by the V-shaped defects known from TEM investigations [6] for the following reasons:

TEM planar views show dark lines with an average separation of 250 Å in agreement with the cross sectional views. The trenches seen with STM have a mean separation of 200–300 Å. Also, the coverage regime where the trenches are created is the same as in the TEM studies. Figure 3 shows that these defect lines often are connected by T-junctions and very rarely intersect each other. This is in contradiction to [7]. The preference for T-junctions indicates that if a V-defect reaches another one running perpendicular, the probability to run further is low. In some partly filled trenches, which are only about two layers deep, we could resolve atomic structure with a smaller layer distance as the surrounding (001) plane [2] which fits to the (111)-platelets proposed for the V-defect. The islands in Fig. 3 which are separated by the trenches are covered by smaller 2D-islands. They have often nucleated at a trench boundary. Islands that nucleated far away to a trench have the same asymmetric length ratio as in the <12 ML case, but if they extend to a trench they are truncated.

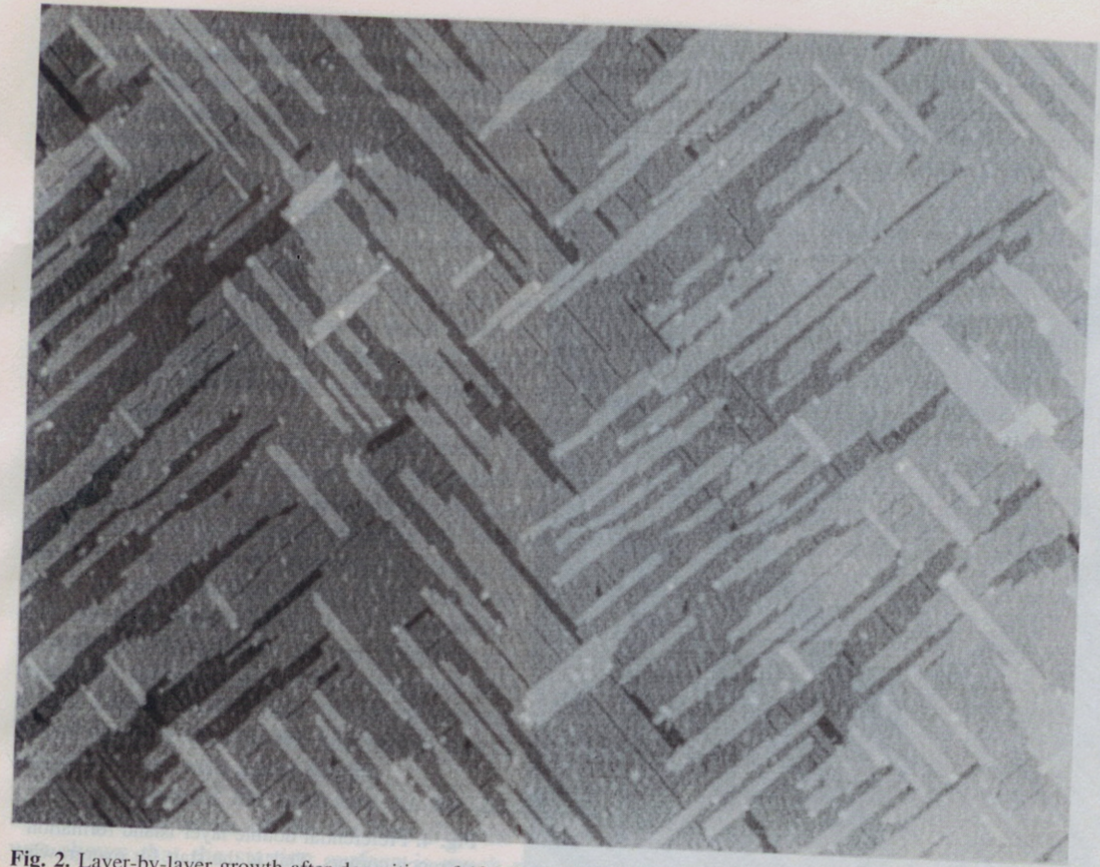

Fig. 2. Layer-by-layer growth after deposition of 12 ML Ge. The islands are extremely anisotropic. (Image size: 2500 Å × 2200 Å)

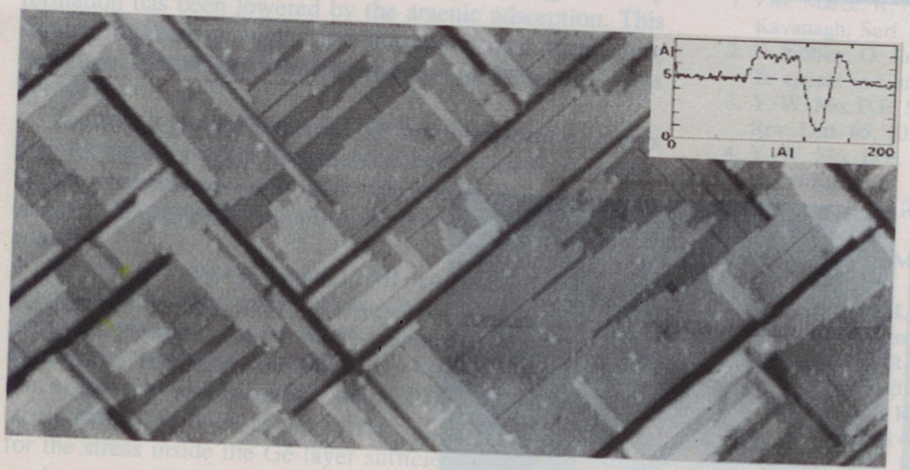

Fig. 3. Network of trenches after deposition of 24 ML Ge. The trenches decorate the V-shaped defects in the Ge-layer (see text). The inset shows a height profile through one of the trenches. (Image size: 2500 Å × 1500 Å)

Extrapolating the mean distance of V-defects necessary for full strain relief to our coverage leads to a separation of 170 Å. The observed average separation is only slightly higher giving rise to the assumption that the strain is almost relieved. Locally this might already be the case, what should increase the possibility that defects become overgrown. Indeed we found numerous examples for such a situation.

In Fig. 4 one can see a branch of a trench running from the lower left to the center of the image and then turning to the upper left. Close to the branch one can see double layer islands on top of the big islands that are separated by the trenches. The center island adjoins three trenches. In this very typical situation the junctions of the trenches act as nucleation centers. The inset in Fig. 3 also reflects this piling up at the boundaries. The resulting double layer islands seem to be the first step for overgrowing a defect. From this tendency to not connecting "bridges" with adjacent "banks" we conclude that these locations are still not free of strain.

We found that most trenches forming the network are connected at both ends with another trench. But there are some exceptions: Fig. 5 images different terminations of trenches.

In the lower part of Fig. 5a and in the center of Fig. 5b there are two trenches visible with a smaller lateral distance that do not pass each other. Trenches running parallel to each other in a smaller distance than about 60 Å are not observed. We assume that the reason for such a termination pair has

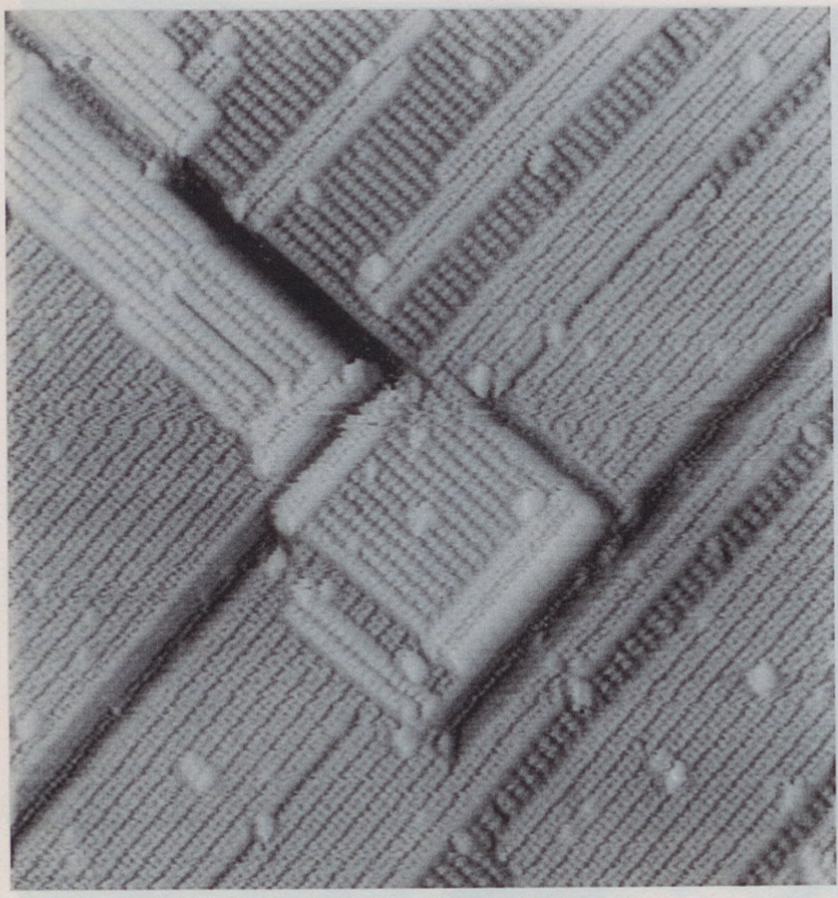

Fig. 4. Preferential double layer island formation at trench corners. This is the start for overgrowing a trench

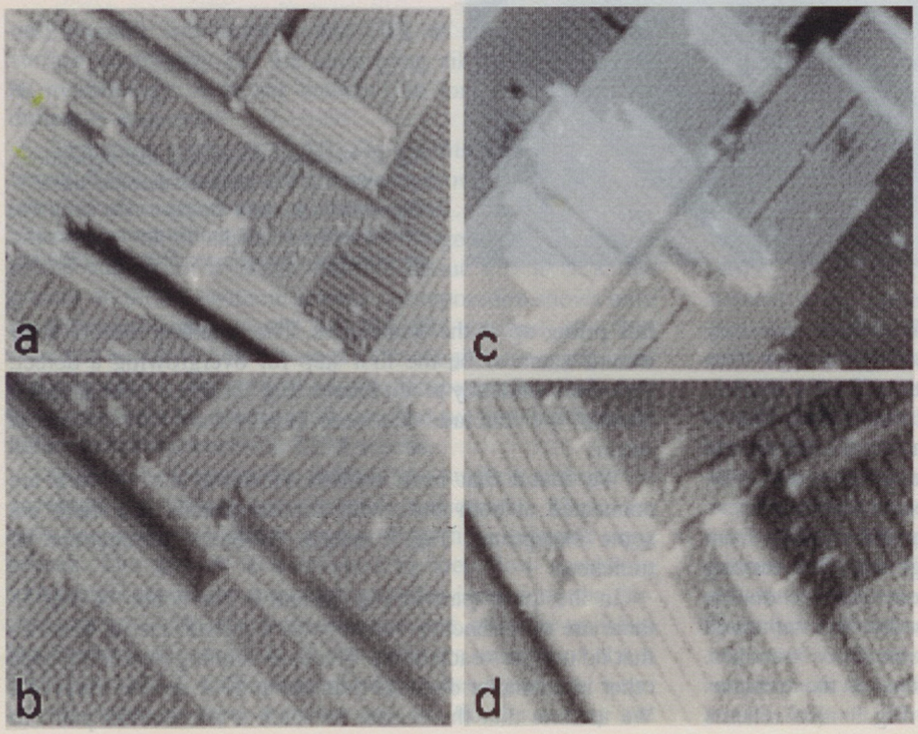

Fig. 5. a, b Trenches prefer to terminate if running in low lateral distance; **c** a partly overgrown trench acts as nucleation center; **d** a stacking fault visible at the surface (step height to the non fitting (2 × 1) island 0.8 Å)

to be found in the strain field range of one V-defect. When the defects nucleate, they are created in such a distance from each other that the local strain is not overcompensated. If a V-defect terminates, a second one can run to this location, to contribute to the local strain relief.

The trenches are created at once between a coverage of 12–16 ML. If the strain is completely relieved by the trenches, their distance should be 113–85 Å at this coverage [6]. LeGoues et al. assume that the V-defect density linearly increases with the film thickness [6–7]. But we neither find any hint for this assumption in their TEM images nor do our 24 ML images show a higher density of V-defects. The number of V-defect seems to remain constant with increasing coverage.

Figure 5c shows a partly filled trench. The filled area has "wings" of small islands that nucleated at the trench boundaries. One can easily imagine the mechanism that leads to such nucleation pinning. Because the boundaries of the trench do not fit into the surrounding lattice, it is very likely that it causes a surface defect which then can act as a nucleation site. Figure 5d shows a terminating defect with a normal (2×1) structure on top. There is a 0.8 Å step between the surrounding and the overgrown (2×1) structure, a step height smaller than the usual monoatomic step. A buried stacking fault in the bulk under this (2×1) domain would produce such a step height.

The presence of the surfactant As has drastic influence on the growth mode of the Ge film. For the first time it was shown that the starting surface is much rougher than assumed up to now. We assume that the energy for step formation has been lowered by the arsenic adsorption. This surface roughening might have the nature of a roughening transition. Further experiments are in progress to clarify this question.

The rough surface structure has more nucleation centers than the nearly perfect flat silicon substrate itself. This may be one contribution to the way the "surfactant" works, because in this stage diffusion is limited by nucleation of small islands.

Up to a coverage of about 12 ML epitaxial Ge layer-by-layer growth is observable. Obviously the film can remain in the pseudomorphic growth mode without forming defects at the surface. The TEM investigation of this system shows that the bulk of the Ge-layer is also free of defects [7]. The tensile stress of the As-layer at the surface [12] may compensate for the stress inside the Ge-layer sufficiently [13].

At a coverage of 24 ML we observed a network of trenches that we identified as caused by V-defects. The energetics of adsorption is such that arriving atoms are driven out of the trenches by diffusion and nucleate in the surrounding area. Further deposition therefore only increases the height of the ajdacent islands but leaves almost all V-defects uncovered up to the coverage where the strain is fully relieved.

The boundaries of the trenches may support strain relief themselves by being distorted. The presence of the defect trenches significantly influences the growth of the film. They confine the growth in separated regions of the surface. The confinement helps suppressing the 3D islanding of the film, because it limits the amount of atoms which can be accumulated to form a 3D cluster in this stage of growth. It could be regarded as "islanding" itself, but the formed "islands" do not grow higher than the mean coverage of the film.

In summary, we have described the surface atomic structure of thin Ge-films that have been grown in the presence of a surfactant. We proposed for the first time that the effect of islanding inhibition may partly be due to the surface reordering of the As covered surface and that the surfactant changes the surface step probabilities anisotropically. We could identify a network of straight trenches as the representation of the so-called V-defects at the surface.

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