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# STM study of the Ge growth mode on Si(001) substrates

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**Abstract**

The Ge growth mode on a Si(001) substrate was examined by scanning tunneling microscopy (STM) on the atomic scale Germanium overlayers on Si substrates exhibited the Stranski–Krastanov growth mode, where the deposited films grew layer-by-layer up to a few ML, followed by the several types of the three-dimensional islands with distinctive facets The phase diagram of the Ge growth was constructed for the Ge coverages from less than 1 ML up to 8 ML at the growth temperatures of 300, 400 and 500°C, examining the STM images Furthermore, annealing effects for the Ge overlayer were also studied to clarify the stability of the islands

## 1. Introduction

Hetero-epitaxially grown films have much potentials to achieve innovative functions for optoelectronic devices A Si–Ge superlattice structure is one of the most attractive candidates However, it poses problems of the non-abruptness and the intermixing at the interface, which modify the band structure [1] The strain induced by a 4 2% lattice mismatch between Si and Ge makes the growth mode complicated, and the Ge-covered surfaces become rough, causing the non-abruptness of the superlattice Up to date, various kinds of structure-analytical techniques, such as low-energy electron diffraction (LEED) [2], Auger electron spectroscopy (AES) [2], reflection high-energy electron diffraction (RHEED) [3,4], X-ray diffraction [5], transmission electron microscopy (TEM) [6], reflection electron microscopy (REM) [7] and scanning tunneling microscopy (STM) [8–14] have been utilized to reveal the growth mode of Ge overlayers on Si substrates The studies classified the growth of Ge films on Si into the Stranski–Krastanov mode, in which the overlayer grows layer-by-layer up to several monolayers, followed by the formation of three-dimensional islands at higher coverages However, the detailed structure of the overlayers and the transition mechanism from the layered growth to the 3D growth are not clear yet In some cases, the transition is not a simple process, and may comprise of several growth stages, including an intermediate phase For example, Mo et al speculated that the Ge hut cluster with four {015} facets was an intermediate phase from the layered growth into the formation of macroscopic clusters with complicated facets [8] But the change of the

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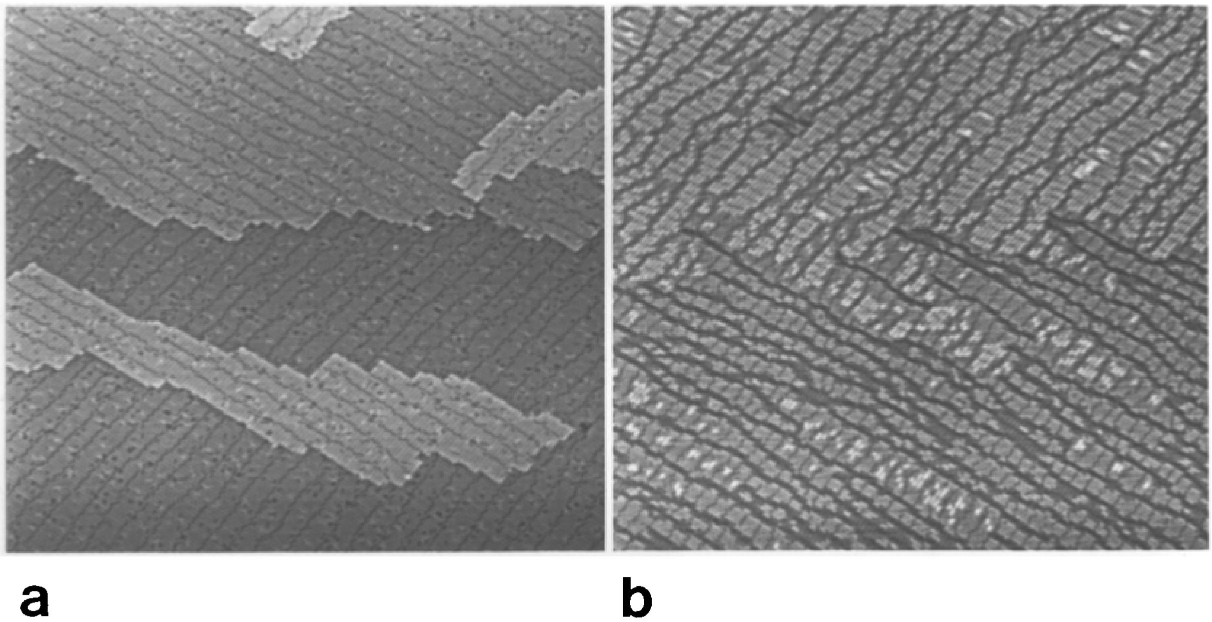

Fig 1 STM images of the Ge overlayers grown layer-by-layer The growth temperature was 500°C Scanning area 960 Å × 910 Å (a) Belt-like structure The deposited amount of Ge was 2 ML (b) Patch-like structure The deposited amount of Ge was 4 ML

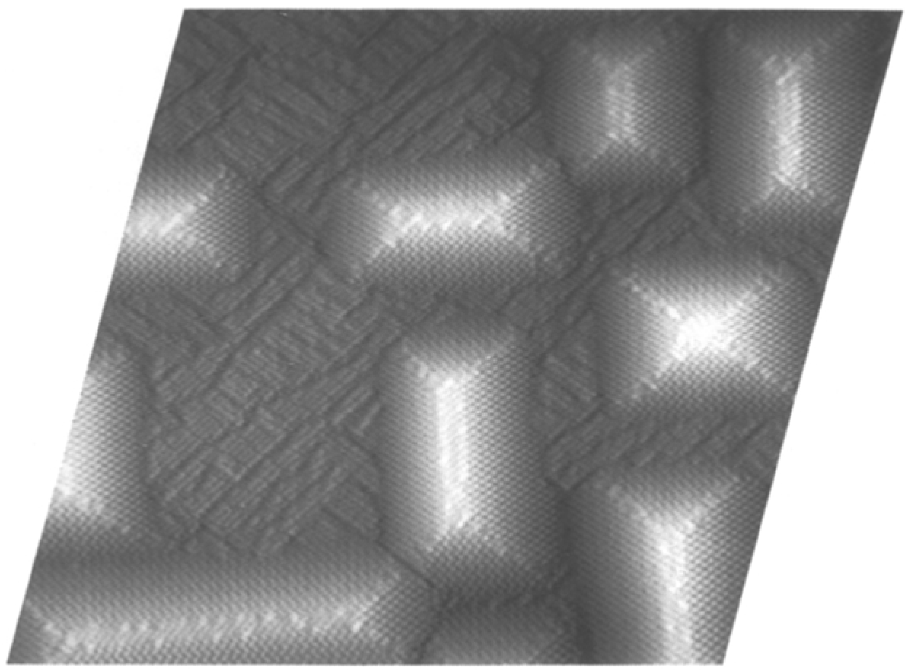

Fig 2 STM image of hut clusters with the {015} facets of Ge on Si(001) The deposited amount of Ge was 5 ML and the growth temperature was 500°C The patch structures surrounded by missing-dimer rows are seen between the hut clusters Scanning area 720 Å × 680 Å

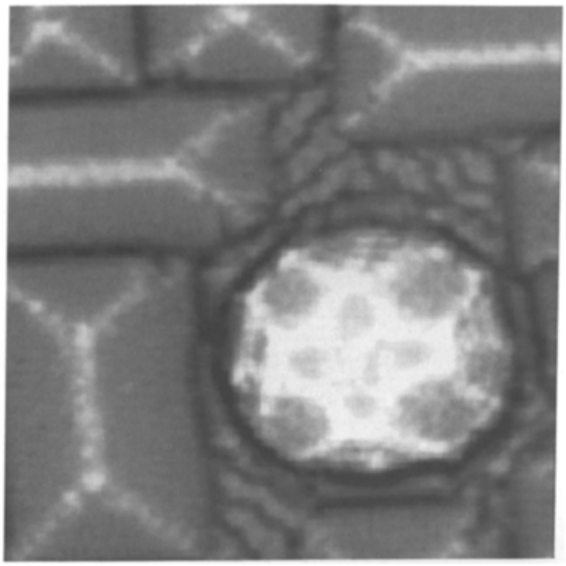

Fig 3 STM image of a dome cluster grown by the deposition of 6 5 ML at 500°C The cluster seems symmetric and has several facet types Scanning area 500 Å × 500 Å

growth mode from the hut clusters into the macroscopic clusters with complicated facets on Si(001) has not been shown into particulars Investigation of the growth phase of the Ge overlayers at various Ge coverages and growth temperatures is indispensable to characterize the growth mode and clarify the growth mechanism This paper will report the surface topography of the Ge overlayers grown on Si(001) substrates up to about 8 ML at the growth temperatures of 300, 400 and 500°C observed by the STM, and also focus on the morphology of the Ge clusters grown three-dimensionally on the substrates

## 2. Experimental

The experiments were carried out in an ultrahigh vacuum chamber with a base pressure of $6 \times 10^{-11}$ Torr with an STM and a Ge deposition source [15] Rectangular pieces cut from an n-type Si(001) wafer with a resistivity of 0 01 Ω cm were

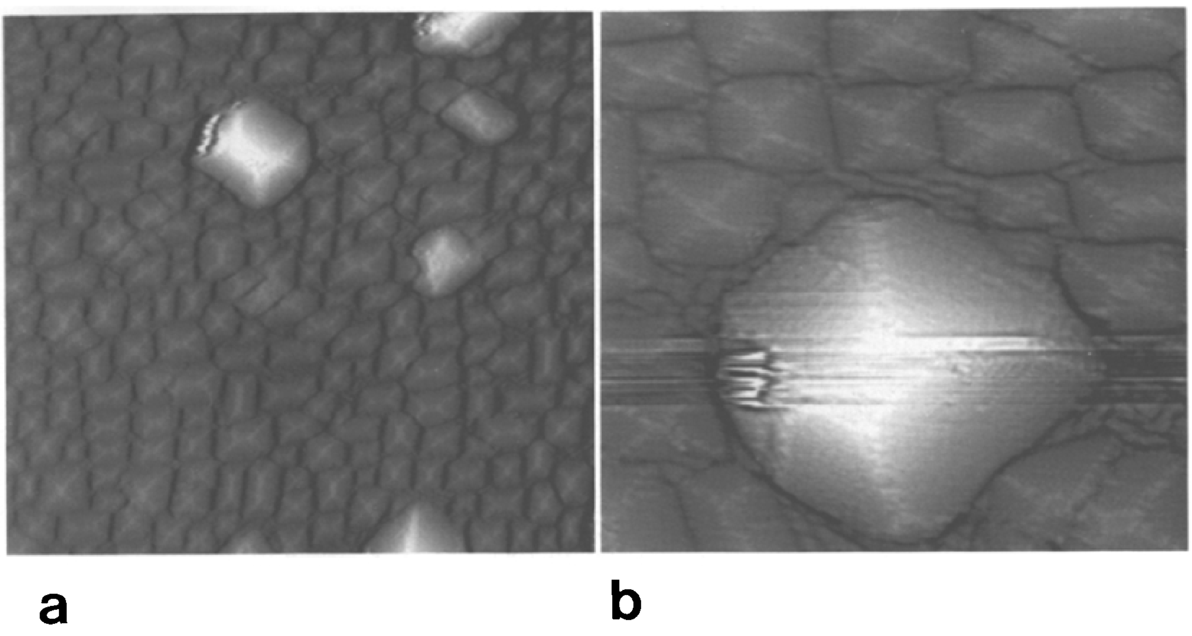


Fig 4 STM image of the nuclei of macroscopic clusters (a) The deposited amount of Ge was 5 ML and the growth temperature was 400°C The hut clusters which covered the whole surface are found between the macroscopic clusters Scanning area 2400 Å × 2300 Å (b) Enlarged STM image of the cluster The cluster has 4 facets, the indices are possibly {113} Scanning area 720 Å × 680 Å

used as substrate for Ge deposition The substrate was chemically cleaned by the Shiraki method [16], then introduced into the STM vacuum chamber, and outgassed at a heat stage in the chamber by resistively heating at 500–700°C After flashing the substrates at about 1200°C for about 15 s, the substrate temperature was gradually cooled and held at 500, 400 or 300°C, then Ge atoms were deposited by heating Ge rods wounded with a tungsten–rhenium filament The deposition rate and the amount were monitored with a quartz thickness monitor The typical deposition rate was 1–5 ML/min After the deposition, the sample was immediately cooled to room temperature and transferred to the STM sample stage to observe the surface topography by the STM The sample deposited by an amount of 5 ML at 400°C was annealed at 500°C for 5 min after the STM observation, and imaged again by the STM to examine the stability of the grown Ge clusters The images were depicted at a tip voltage of 2 0 V and tunneling currents of 0 2 to 1 nA

## 3. Results and discussion

The Ge overlayers on Si(001) grow layer-by-layer at less than several ML At Ge coverages less than 1 ML the deposited Ge atoms dimerize on the Si(001) surface and form chain-like rows showing a c($4 \times 2$) and a p($2 \times 2$) reconstruction [10] In spite of the 4 2% lattice mismatch between Ge and Si, there is no distinctive difference from the Si homoepitaxial growth except the strong buckling However, at the coverage higher than 1 ML, the missing dimer rows are introduced, exhibiting belt or patch structures to release the strain piled up along the dimer row Fig 1a shows the Ge-layered growth with belt structures at 2 ML at 500°C, the step and the two-dimensional islands are seen partially The dark

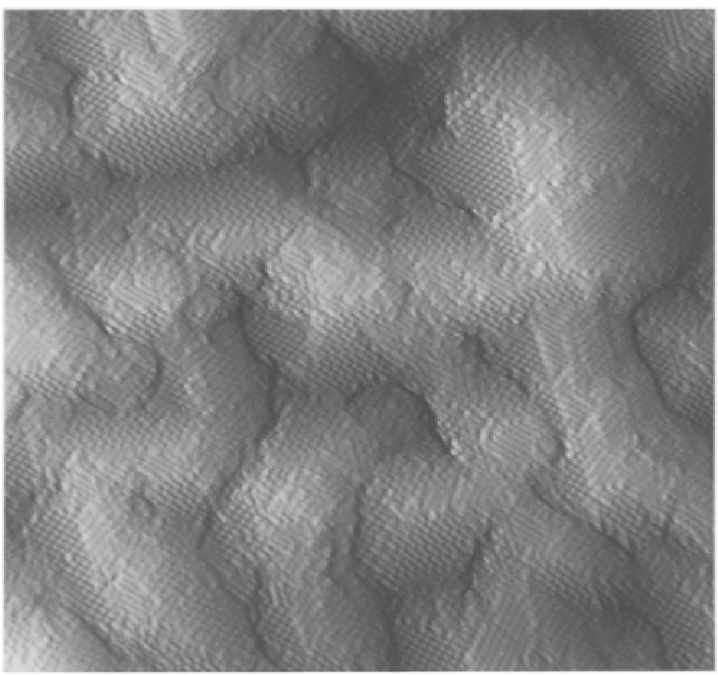

Fig 5 STM image of the fused hut clusters The deposited amount of Ge was 8 ML and the growth temperature was 300°C The dimer rows on the (001) surface can be observed on the top Scanning area 720 Å × 680 Å

lines of the missing dimer rows run with spacings of 8–11 times the lattice constant At the higher coverage of 4 ML the overlayer exhibits patch structures surrounded by missing-dimer rows and trenches, which cross at a right angle owing to the 90° rotation of the dimer rows on the single-atomic overlayer, see Fig 1b

Fig 2 shows the hut clusters with 4 facets of the {015} planes grown 5 ML at 500°C The plane indices were determined by measuring the slope angles to the substrate and the orientation of the principal axes The STM image exhibits the regular zigzag patterns with a 2 × 1 reconstruction on the {015} and the dimer rows on the top (001) surface of the hut clusters [8–14] The patch structures are also seen in flat spaces between the clusters

When almost the whole surface is covered with the hut clusters by the increased amount of Ge deposition, other cluster types larger than the hut clusters are found Fig 3 shows a dome cluster on the Ge overlayer grown with 6 5 ML deposition at 500°C It looks four-fold symmetric, and the surface seems to be composed of the (001), {015} and {113} facets, estimated from the slope angles and the orientations The hut clusters do not seem to grow larger because the contact of the clusters on the base plane impedes further growth Thus, the growth mode changes from the hut cluster to the dome cluster On the other hand, at the growth temperature of 400°C the macroscopic clusters with 4 facets of the {113} planes grow at coverages higher than 5 ML, see Fig 4 [8] The symmetrical axis of the macroscopic cluster is rotated 45° with respect to that of the hut clusters Several hut clusters coalesce with the neighbors rotating the boundaries 45° They are possibly the nuclei of the macroscopic clusters

At the growth temperature of 300°C, at the high coverage of 8 ML, the hut clusters coalesce with each other and fuse to form a rugged surface after the whole surface is covered with the clusters, see Fig 5 The regular zigzag patterns on the {015} facets and the dimer rows on the top still remain, and there are no other facets, even at the thick coverage At the low temperature of 300°C the {015} facets in the strained region close to the Ge–Si interface are stable compared with

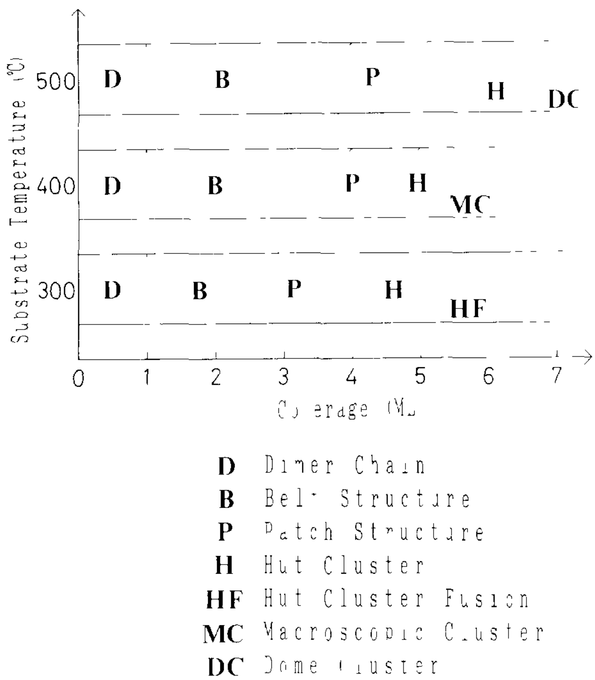


Fig 6 Phase diagram of the Ge growth mode on the Si(001) substrate at 300, 400 and 500°C It is constructed from the STM images obtained in this study The dashed lines roughly indicate the coexisting range of two phases at both sides of the lines

the {113} facets of the macroscopic clusters Since the {015} consists of two-dimer rows on the small (001) terraces and single-atomic height steps, the strain piled up along the dimer row is easily released at the step edges [14] At higher temperatures the {113} facets of the macroscopic clusters are energetically favorable The strain may partially relax inside or under the clusters because the facets in the top region of large macroscopic clusters are far away from the interface where the strain seems concentrated

The detailed growth mode with the transition from 2D- to 3D-islands formation depends on the growth temperature, as stated above Fig 6 shows the phase diagram of the Ge growth mode on the Si(001) substrates, which summarizes this study The morphology of the Ge clusters changes drastically after the formation of the hut clusters The critical thickness of Ge from two-dimensional to three-dimensional growth, that is from the patch

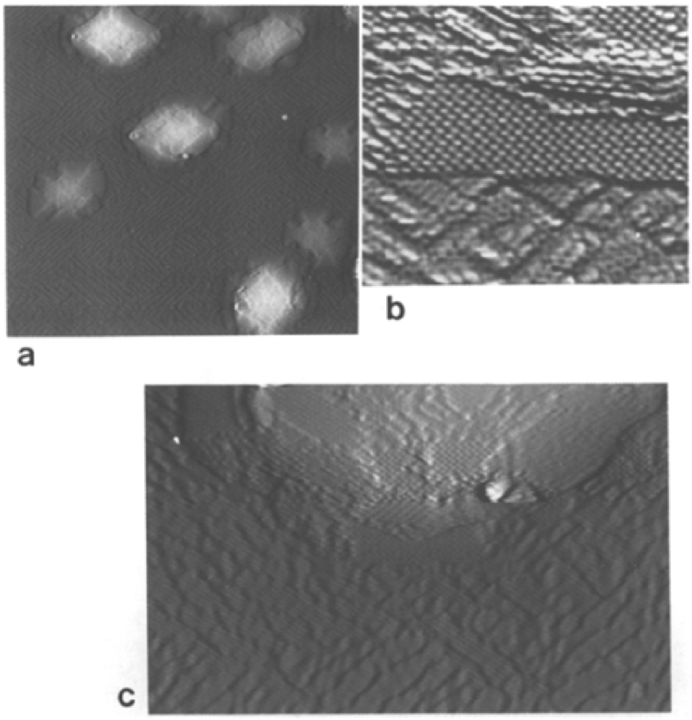


Fig 7 (a) STM image after the annealing of the sample shown in Fig 4 at 500°C for 5 min Other types of macroscopic clusters with complicated facets grew The hut clusters disappeared and the patch structure appeared again between the macroscopic clusters Scanning area 2400 Å × 2300 Å (b) Image of the foot of the cluster The zigzag patterns on the {015} surface are clearly recognized Scanning area 240 Å × 200 Å (c) Enlarged image of a half of the cluster Scanning area 710 Å × 450 Å

structure to the hut clusters, is more than 3 ML, and slightly increases with the temperature Si and Ge atoms near the interface may intermix at 500°C and the lattice mismatch can be reduced a little to increase the thickness

For the 5 ML Ge overlayer grown at 400°C annealing effects for 5 min at 500°C were also investigated As shown in Fig 7, the macroscopic clusters disappear and new types of complicated clusters grow, which have the {015} facets on the foot of the clusters, the {113} facets on the breast, and the $2 \times 1$ reconstructed (001) surface with many steps on the top The hut clusters disappear by the annealing as if the macroscopic clusters absorb the hut clusters, and then are transformed into the complicated clusters After the hut clusters' disappearance, the patch structures with missing-dimer rows reappear between the complicated clusters The overlayer with the patch structures, whose thickness is perhaps 3 ML, may be strongly bound to the substrate, while the hut clusters may be loosely bound to the substrate and then are easily transformed by the annealing The reappearance of the {015} facets on the foot of the clusters after the annealing indicates the stability of the {015} surface in the region close to the interface The growth mode of Ge on the (015) substrate is interesting where the critical thickness from 2D to 3D growth increases drastically The experimental results are published elsewhere [14]

## 4. Conclusion

Ge overlayers grown at the growth temperatures of 300, 400 and 500°C up to the Ge coverages of 8 ML on the Si(001) substrates were observed by the STM The phase diagram of the Ge growth mode was constructed from the STM images obtained in this study It exhibited the temperature dependence of the growth mode, particularly of the formation of the three-dimensional clusters Annealing effects of the macroscopic clusters were studied, and the stability of the {015} facets in the region close to the Ge–Si interface was indicated

## 5. Acknowledgement

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