Strain-induced dimer adatom stacking fault structures of germanium on Si(111)-($\sqrt{3}\times\sqrt{3}$)$R30°$:B observed by scanning tunneling microscopy

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The growth and the atomic structure of the Ge on the Si(111)-($\sqrt{3}\times\sqrt{3}$)R 30° surface are investigated by scanning tunneling microscopy. The coexistence of the ($\sqrt{3}\times\sqrt{3}$)R 30° and the $c(2\times4)$ reconstruction at the Si-substrate is discussed. Germanium on silicon, usually indistinguishable from the silicon is identified on the boron induced ($\sqrt{3}\times\sqrt{3}$)R 30° surface using the difference in reconstruction of the substrate and epitaxial material. The germanium deposit shows a dimer adatom stacking fault-like structure while the substrate still remains ($\sqrt{3}\times\sqrt{3}$)R 30° reconstructed. A significant boron diffusion is only observed after annealing at 480 °C, which converts the island surface into a ($\sqrt{3}\times\sqrt{3}$)R 30° reconstruction.

The epitaxial growth of germanium on different silicon surfaces has been investigated intensively for some time.[1,2] But even investigations by means of scanning tunneling spectroscopy can not necessarily be a tool to distinguish between Si and Ge. For the preparation of quantum wires or quantum dots we need a method which is able to identify the different species on an atomic scale. In order to improve the crystalline quality of Si/Ge heterostructures (e.g., reduce the number of dislocations), a detailed knowledge of the first stage of the epitaxial growth at the interface is necessary. On the other hand it is interesting to determine the inherent properties of the Ge deposit by comparing the growth on differently reconstructed surfaces, e.g., on the Si(111)-(7×7) and on the Si(111)-($\sqrt{3}\times\sqrt{3}$)R 30° surface.

The chemical properties of the Si adatoms on the Si(111)-($\sqrt{3}\times\sqrt{3}$)R 30°:B surface differ from those on the Si(111)-(7×7) surface.[3] The ($\sqrt{3}\times\sqrt{3}$)R 30° reconstruction on Si(111) can be induced by the group-III elements (B,[4,5] Al,[6] Ga,[7] In[8]). But only on the boron-induced Si(111)-($\sqrt{3}\times\sqrt{3}$)R 30° surface the top layer is suggested to consist of silicon, completely, since the Si–B bonds are too short to be stable in the usual T_4 adatom geometry.[4,5,9,10] Therefore the B atoms are supposed to be placed directly below the T_4 Si-adatoms in the B_5 position.

The boron-induced Si(111):B-($\sqrt{3}\times\sqrt{3}$)R 30° surface is not only of fundamental interest but also interesting for semiconductor technology, e.g., it can be used in connection with a scanning tunnel microscope-tip (STM) to realize the tunnel diode effect on the atomic scale.[11,12] The Ge/Si(111):B system, on the other hand can be applied for δ-doped heterostructures and Ge/Si superlattices.

We have studied the nucleation behavior and the atomic structure of the germanium epilayer at the interface to the Si(111):B($\sqrt{3}\times\sqrt{3}$)R 30° substrate. Our results should clarify what kind of superstructure the Ge deposit forms on the Si(111)-($\sqrt{3}\times\sqrt{3}$)R 30° surface and at which temperature a significant diffusion of boron from the substrate to the islands takes place. If the temperature for the boron diffusion is sufficiently high so that the Ge deposit does not form a $\sqrt{3}$ superstructure we are able to achieve material contrast for the germanium arranged in one and two dimensional structures. The experiments were carried out in a dual-chamber ultra high vacuum system (base pressure 10^{-10} mbar) containing the Ge-Knudsen-source heated by electron bombardment and the microscope[13] with a tungsten tip. After transfer via load lock the samples [0.002 Ω cm boron ultrahigh vacuum doped Si(111) wafers] were degassed (10 h at 500 °C and 15 min at 800 °C), and their native oxide was removed by flashing up to 1250 °C for several times. Before filling, the evaporator made of graphite was carefully outgassed for several hours at about 1800 °C. The growth rate was three monolayers per minute (one monolayer = 7.84×10^{14} atoms).

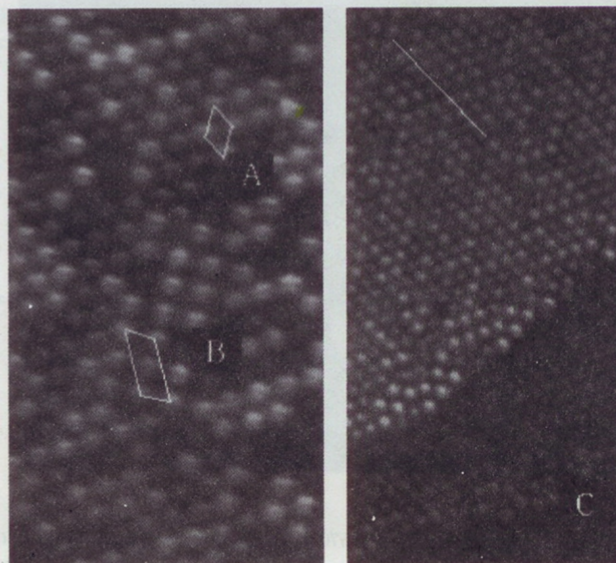

FIG. 1. Si(111):B substrate used for Ge epitaxy ($\sqrt{3}\times\sqrt{3}$)R 30° and $c(4\times2)$ reconstructed (marked by A and B, respectively). The $c(4\times2)$ reconstruction occurs at ($\sqrt{3}\times\sqrt{3}$) domain boundaries and inside the domains. All adatoms are placed at T_4 sites. DAS structures are only occasionally found at step edges (marked by C). The scans are about 40 Å×80 Å and 70 Å×140 Å, respectively.

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The STM topographs were obtained in the other chamber after cooling down the sample to room temperature (sample bias + 1.5 V and tunneling current about 1 nA).

Figure 1 shows two STM topographs of the well prepared substrate without any islands. We can find "dark" and "bright" atoms arranged in small domains. All these atoms are silicon but below the "dark" ones, boron atoms are placed in the B_5 site.[4,5,9,10]

In general, the surface has a $(\sqrt{3}\times\sqrt{3})R\,30°$ periodicity (marked by A). The stacking of the adatoms at the $(\sqrt{3}\times\sqrt{3})$ domain boundaries forms the $c(4\times2)$ structure, but there are also $c(4\times2)$ unit cells inside the domains (marked by B).

In both structures, $(\sqrt{3}\times\sqrt{3})R\,30°$ and $c(4\times2)$, the Si adatoms are placed at T_4 sites, but in the ideal $(\sqrt{3}\times\sqrt{3})R\,30°$ reconstruction no dangling bonds exist whereas in the $c(4\times2)$ unit cell two dangling bonds in the restatom layer occur.

For our observation that the $c(4\times2)$ reconstructed area is $(4\pm1)\%$ for each topograph we do not find a clear explanation. Further investigation should clarify if the kinetics of the domain formation, relatively homogeneously distributed impurities or the variations in the distribution of the boron atoms perpendicular to the surface are the dominant process responsible for this behavior.

The step edges are usually straight and consist mainly of short ordered domains of (2×2) arrangements up to 20 Å wide. Often the $\sqrt{3}$ structure reaches the step edges. Only occasionally dimer adatom stacking fault (DAS)-like structures are found at the step edges. They are at maximum one unit cell wide and cover up to 10% of the edge.

Figure 2 shows a STM topograph of the surface after germanium growth of 0.4 monolayers at 420 °C. The islands consist of elements with diameter from 20 to 80 Å, and in general have irregularly shaped step edges. Only a few islands reconstructed in a DAS structure [mostly (5×5)] are triangular. At the other islands a mixture of structures containing (2×2), (3×3), (5×5), (7×7) and other reconstructions occurs. But the $(\sqrt{3}\times\sqrt{3})R\,30°$ reconstruction we only find at the substrate. Since the presence of boron also causes a $(\sqrt{3}\times\sqrt{3})R\,30°$ reconstruction on the Ge-epilayer (shown in Fig. 3), no noticeable boron diffusion takes place up to 420 °C.

At the step edges, in a range of about two or three (5×5) unit cells we find the same structures than at the islands, no $\sqrt{3}$ reconstruction is observed (see Fig. 2). Moreover, near the step edges the concentration of islands is depleted. That means the species of the stripe at the step edge and of the islands are the same.

Bulk diffusion coefficients of Ge in Si predict negligible interdiffusion below 600 °C.[14] Auger spectroscopy[15] and Rutherford backscattering results[16] indicate no alloying between Ge and Si in the submonolayer region at our growth temperature of 420 °C. Therefore we can conclude the islands and the stripe along the step edge reconstructed in the same manner as the islands which is about 50 Å wide consist nearly exclusively of germanium. At the step edge of the substrate Si has formed up to 10% DAS structures, too, (see

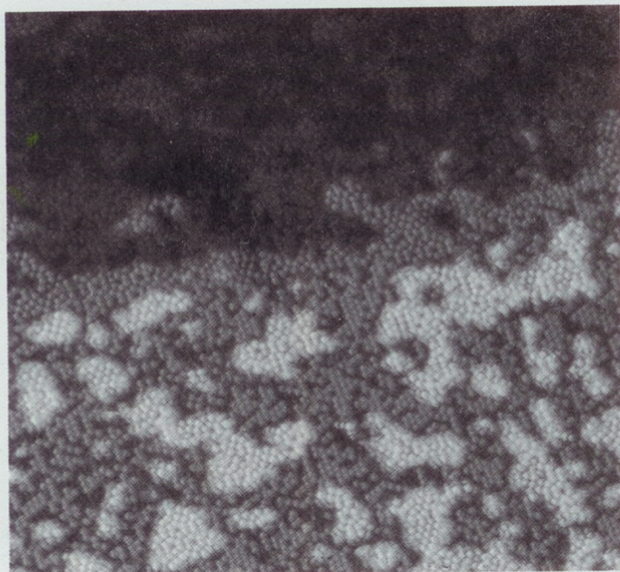

FIG. 2. STM topograph (750 Å × 670 Å) of the surface after the Ge growth of 0.8 monolayer at 420 °C. The islands have an irregular shape in general. Only those few islands which are (5×5) reconstructed are triangular (see at the bottom of the topograph). We have found a mixture of reconstructions on the islands but not the $(\sqrt{3}\times\sqrt{3})R\,30°$ structure as on the substrate. At the step edge (in the upper part of the topograph) we can distinguish between the deposit and the substrate material clearly because of their different reconstructions.

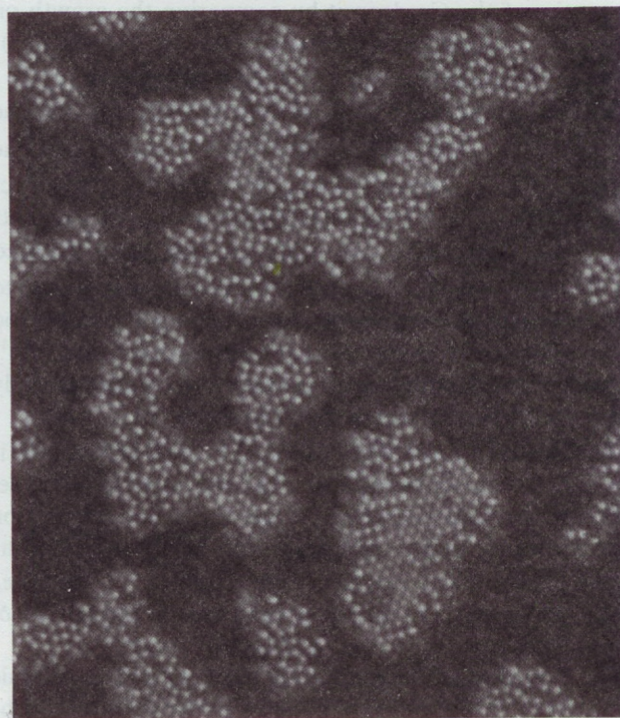

FIG. 3. The surface shown in Fig. 2 after annealing at 480 °C for 15 min. At the islands the $(\sqrt{3}\times\sqrt{3})R\,30°$ reconstruction occurs and at the substrate the $c(4\times2)$ structure appears again indicating that boron diffusion takes place. (scan size ~ 500 Å × 500 Å).

discussion of Fig. 1) and therefore the determination of the interface between Si and Ge is accurate at least within 20 Å.

Note, in Fig. 2 the $c(4\times2)$ reconstruction in the substrate layer just only occurs on the Ge stripe at the step and on the islands and not on the Si substrate. Therefore we may assume that this structure in the substrate layer is a preferential site for nucleation.

For further investigations the step edge and the islands consisting of Ge could be used to study tunneling spectra of Si and Ge in detail. The more important conclusion, however, is that the deposit is arranged at the step edges like a wire in atomic dimensions, and STM can be used to study the growth conditions for preparing low dimensional systems.

After annealing the sample shown in Fig. 2 at 480 °C for 15 min we get larger, more ordered islands with straighter edges (see Fig. 3).

The $(\sqrt{3}\times\sqrt{3})R\,30°$ reconstruction on many islands indicates that the boron diffusion takes place at temperatures between 420 and 480 °C. The $c(4\times2)$ structures now present on the substrate may be another indication for boron diffusion.

It should be noted that the amount of "bright" atoms is significantly higher on the Ge islands than on the substrate. if the model for the Si(111)-$(\sqrt{3}\times\sqrt{3})R\,30°$ surface[4,5,9,10] is also valid for Ge, there is only a small amount of boron in the B_5 site under the islands.

In order to compare the Ge growth on Si(111)-(7×7) and $(\sqrt{3}\times\sqrt{3})R\,30°$ surfaces we have determined the denuded zone of islands around the step edges on average which is nearly equal to the distance between the islands. For Si(111)-$(\sqrt{3}\times\sqrt{3})R\,30°$ this length is (120 ± 40) Å at 420 °C and (200 ± 60) Å after annealing at 480 °C. In the case of Ge growth on Si(111)-(7×7) this is 120 Å at 420 °C and 800 Å at 500 °C (see Ref. 2). These data are obtained from nine micrographs each with an area of about 1250 Å × 1250 Å. The derivation of the data at the higher temperatures can be explained by the different preparation: The sample with the $(\sqrt{3}\times\sqrt{3})R\,30°$ structure was post-annealed at 480 °C and in the other case Ge was directly grown on Si(111)-(7×7) at 500 °C.

These data suggest the migration and the nucleation behavior of Ge on Si(111)-(7×7) and $(\sqrt{3}\times\sqrt{3})R\,30°$ are comparable. Although the islands are differently shaped the kinetics of islands formation is similar. More data are necessary to compare the individual processes (migration, nucleation, growth, etc.) which involved into the molecular-beam epitaxy growth.

At higher Ge coverages the (5×5) areas become larger and larger and above five monolayers we obtain 3D-islanding. Thus, we have shown that Ge grows on the $(\sqrt{3}\times\sqrt{3})R\,30°$-reconstructed Si(111) surface in the Stranski–Krastanov-mode, similar to the Ge-growth on the (7×7)-reconstructed Si(111) surface (see Ref. 2) and on the Si(001) surface (see Ref. 13).

In summary we can state, the DAS structure at the surface is an inherent property of the germanium deposit grown under compressive strain. Therefore regions of Si and Ge can be distinguished up to growth temperatures of about 450 °C. It is shown that differently reconstructed materials can be used to study the growth conditions for preparing low dimensional systems by STM. But to understand the growth process and the atomic structure of Ge on Si completely by means of physical terms, further investigations are necessary.

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[1] Y. W. Mo, D. E. Savage, B. S. Swartzentruber, and M. G. Lagally, Phys. Rev. Lett. **65**, 1020 (1990).

[2] U. Köhler, O. Jusko, G. J. Pietsch, B. Müller, and M. Henzler, Surf. Sci. **248**, 321 (1991).

[3] P. Avouris, I.-W. Lyo, F. Bozso, and E. Kaxiras, J. Vac. Sci. Technol. A **8**, 3405 (1990).

[4] I.-W. Lyo, E. Kaxiras, and P. Avouris, Phys. Rev. Lett. **63**, 1261 (1989).

[5] R. L. Hendrick, I. K. Robinson, E. Vlieg, and L. C. Feldman, Phys. Rev. Lett. **63**, 1253 (1989).

[6] R. J. Hamers and J. E. Demuth, Phys. Rev. Lett. **60**, 2527 (1989).

[7] J. E. Zegenhagen, J. R. Patel, P. Freeland, D. M. Chen, J. A. Golovchenko, P. Bedrossian, and J. E. Northrup, Phys. Rev. B **39**, 1298 (1989).

[8] J. Norgami, S. Park, and C. F. Quate, Phys. Rev. B **36**, 6221 (1987).

[9] P. Bedrossian, R. D. Meade, K. Mortensen, D. M. Chen, J. A. Golovchenko, and D. Vanderbilt, Phys. Rev. Lett. **63**, 1257 (1989).

[10] P. Bedrossian, K. Mortensen, D. M. Chen, and J. A. Golovchenko, Phys. Rev. B **41**, 7545 (1990).

[11] P. Bedrossian, D. M. Chen, K. Mortensen, and J. A. Golovchenko, Nature **342**, 259 (1989).

[12] I.-W. Lyo and P. Avouris, Science **245**, 1369 (1989).

[13] J. E. Demuth, R. J. Hamers, R. M. Tromp, and M. E. Welland, J. Vac. Sci. Technol. A **4**, 1320 (1986).

[14] G. J. Fisanick, H.-J. Gossmann, and P. Kuo, Mat. Res. Soc. Symp. Proc. **102**, 25 (1988).

[15] H.-J. Gossmann, L. C. Feldman, and W. M. Gibson, Surf. Sci. **155**, 413 (1985).

[16] P. M. J. Maree, K. Nakagawa, F. M. Mulders, J. F. van der Veen, and K. L. Kavanagh, Surf. Sci. **191**, 305 (1987).