PHYSICAL REVIEW B VOLUME 51, NUMBER 19 15 MAY 1995-I

Domain-boundary-induced metastable reconstructions during epitaxial growth of Si/Si(111)

Y.-N. Yang
Department of Physics, University of Maryland, College Park, Maryland 20742-4111

E. D. Williams
Department of Physics and Institute for Physical Science and Technology, University of Maryland, College Park, Maryland 20742-4111

(Received 13 October 1994; revised manuscript received 23 January 1995)

The formation of 5×5 and 2×1 reconstructions of Si(111) has been monitored during homoepitaxial growth. We show that these metastable reconstructions are induced by the domain boundaries. We demonstrate this by contrasting the growth structures, in the submonolayer regime, on substrates with different densities of domains. All islands nucleated on the domain-boundary-free substrate are found to have 7×7 structure, while equal amounts of 7×7, 5×5, and 2×1 are observed in the islands in the substrate with large numbers of domain boundaries.

INTRODUCTION

That metastable reconstructions can form during homoepitaxial growth on Si(111) after several monolayers of growth has been known for quite some time. Using low-energy electron diffraction (LEED), Hoegen, Falta, and Henzler reported that more than 50% of the surface was covered by the 5×5 reconstruction after 10 ML of deposition.[1] The growth of islands which have partial 5×5 reconstruction has also been observed using scanning-tunneling microscopy (STM).[2] More recently, 2×1 reconstruction has been observed by STM on Si(111) following 6.5 ML deposition.[3,4] However, it is not clear what causes these metastable structures to form. An important feature of these observations is that metastable reconstructions were often observed under growth conditions where perfect layer-by-layer growth is achieved, i.e., where sufficient diffusion is available to allow atoms to move to the lowest-energy configuration.[3] This fact strongly suggests that the formation of these reconstructions is unlikely to be caused solely by limited kinetics. Rather, their formation is a result of energetics associated with growth. There are two obvious possible explanations. The first is that, at high coverage, many domain boundaries are present on the surface which could cause the formation of metastable reconstructions. The second is that after long-time deposition, impurities could accumulate on the surface which could also cause the observed metastable structures to form.

In this work, we demonstrate, using scanning tunneling microscopy, that the formation of 5×5 and 2×1 reconstructions during growth is induced by domain boundaries on the Si(111) surface. We demonstrate this by showing that the 5×5 and 2×1 reconstructions can be found in the islands nucleated at domains boundaries following submonolayer deposition of Si. We further show that we can change the percentage of islands with metastable reconstructions by artificially changing the density of domain boundaries on the substrate. Finally, we firmly establish the domain boundary as the cause for the formation of 5×5 and 2×1 reconstructions during homoepitaxial growth on Si(111), therefore eliminating impurity and kinetics as possible causes, by showing that even on the same surface the metastable reconstructions are strongly correlated with the existence of domain boundaries.

EXPERIMENT

The experiments were performed in an UHV system with a base pressure of 2×10^{-11} Torr, equipped with a homemade scanning tunneling microscope. Nominally flat Si(111), *n*-doped wafers, $15\times3\times0.4$ mm^3 in size, were used as samples without any chemical precleaning. Heating was achieved resistively with dc current. Clean Si(111) surfaces were obtained by flashing to 1250 °C for 1 min, after degassing at 700 °C. The samples were then quickly cooled to 900 °C. From 900 °C to below 250 °C, the samples were either quenched with a cooling rate of ~100 °C/s to create a substrate with a large density of domain boundaries, or cooled down slowly with a rate of ~0.5 °C/s to obtain a substrate with few domain boundaries. One of the key processes in preparing the substrates, as we will show, is to create large terraces by heating the sample at 1200 °C with dc current in the down-step direction. The details of the creation of large terraces through electromigration have been described previously.[5,6] Another Si wafer, placed ~2 cm from the sample, is used as the Si deposition source. The pressure during deposition was less than 3×10^{-11} Torr. The coverage of the deposition will be expressed in units of double layers (DL's) of Si(111), where 1 DL is equal to 1.36×10^{15} atoms/cm^2. The temperatures of the sample and the source were measured using an IR pyrometer.

RESULTS

Figure 1(a) shows an image following deposition of 0.03 DL (10 s) of Si on a substrate at 420 °C that was slowly cooled from 900 °C. Pairs of steps in the image were created by stopping at 1100 °C for 3 min when the sample was cooled from 1200 °C to 900 °C with the current in the up-step direction to increase the sizes of the terrace.[5–9] The sawtooth appearance of step edges in the image is due to the misalignment of the step directions to any of the high-symmetry directions, and represents the attempts of the steps to lower their energies by breaking up into step segments that are along the $[\bar{1}\bar{1}2]$ and $[\bar{2}11]$ directions, respectively. The small white features in the image have been identified in smaller-area scans as due to Si islands. Clearly, there are two general types of island, those arranged in lines and those arranged randomly. Islands nucleated at the domain boundaries appear as lines of white dots. Such lines of islands serve as an efficient domain boundary marker: domain boundaries can be identified even in large-area scans like the one shown in Fig. 1(a). The alignment of the corners of the sawteeth of the step edges with the ends of domain boundaries is such that the length of the boundary connecting the steps is minimized. The regions on the substrate bounded by domain boundaries and steps are 7×7 single domains. The island nucleation in these domain-boundary-free regions are random, and some of the islands found in this region, as we will show, have multiple layers.

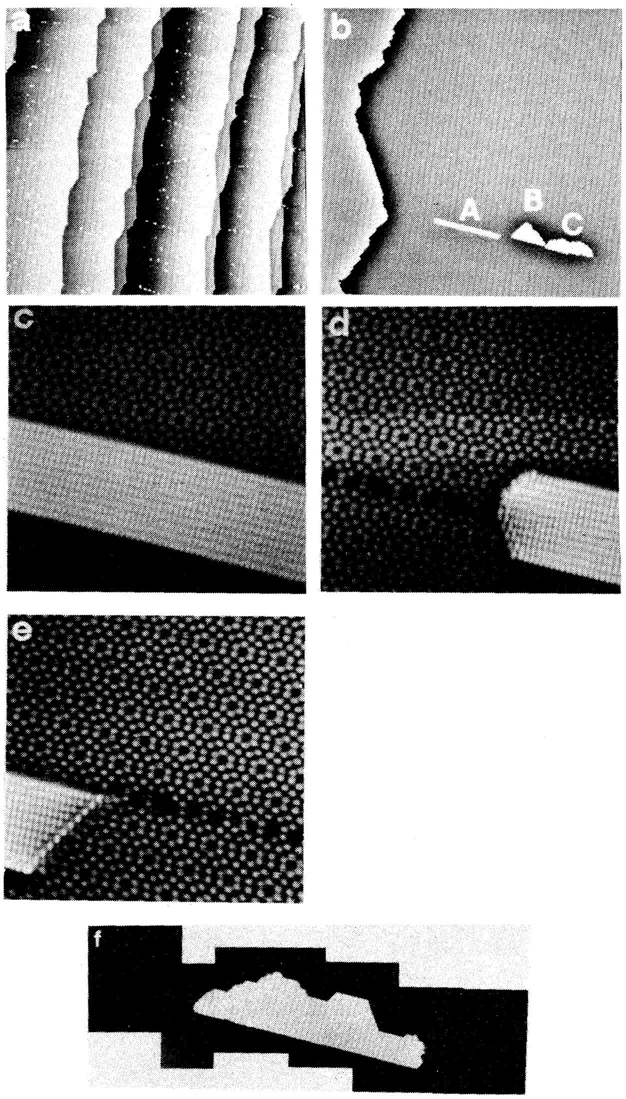

FIG. 1. (a) STM images of area 3000×3000 nm^2 after deposition of 0.03 DL of Si showing that islands nucleate preferentially at domain boundaries and randomly nucleate within single domains of 7×7 reconstruction. The sample temperature during deposition was 420 °C and the deposition rate was 0.003 DL/s. (b) Smaller-scale image (450×450 nm^2) showing three islands at a domain boundary. Island A has a 2×1 reconstruction, while islands B and C have 7×7 reconstructions. (c) Atomically resolved image of a middle section of island A showing the 2×1 reconstruction, and interfaces with the surrounding 7×7 reconstruction in the substrate. (d) and (e) Images of the two ends of the island A and the domain boundaries in the substrate. (f) A mosaic image of a 5×5 island at a domain boundary.

Figure 1(b) shows a smaller scale image (450×450 nm^2) of three islands nucleated at a domain boundary. Even though, at this scale, no atomic features are resolvable, it is clear from the image that island A, measuring 6.6×70nm^2, has a darker gray scale than that of islands B and C, indicating that it has a lower height (islands B and C have the same apparent height as the step height on the left of the image, and the background subtraction done on the image made it appear otherwise). The atomically resolved image of Fig. 1(c) reveals that island A has a 2×1 reconstruction, while islands B and C consist of 7×7 reconstruction (not shown). Figures 1(d) and 1(e) show the two ends of island A and the domain boundaries in the substrate. A dual image (not shown) that probes the filled and empty states simultaneously shows that the 2×1 structure is identical to those observed on cleaved Si(111).[10–12] Thus the apparent rectangular lattice in Figs. 1(c)–1(e) ($+2v$ sample bias, empty state) represents only half of the atoms in the 2×1 structure, and the other half can only be probed with negative bias voltage. The π-bonded chain model of the 2×1 structure involves only the relaxation of the surface atoms, while the 7×7 and 5×5 structures involve decoration of adatoms on the surface. Therefore, geometrically, the 2×1 island is lower in height than that of the 7×7 and 5×5 islands, which may be responsible for the lower height for the 2×1 island in our STM images. It is also interesting to note that the structures of the two parallel interfaces between the 2×1 island and the 7×7 island in the substrate are different.[4] Figure 1(f) shows a mosaic image of an island with 5×5 reconstruction, again nucleated at a domain boundary of the substrate.

We have grown different amounts of Si (0.02 DL $< \theta < 0.5$ DL), at different temperatures (390–510 °C) with different deposition rates (0.001 DL/s–0.15 DL/s) on substrates similar to that shown in Fig. 1(a). Even though most of the islands grown on the substrate in the submonolayer regime have a 7×7 reconstruction, we have always been able to find 2×1 and 5×5 islands at the domain boundaries. In constrast, the islands nucleated in the region with no domain boundaries always have 7×7 reconstruction in their first layer. Such an observation strongly suggests that the formation of these metastable reconstructions is correlated with the domain boundaries in the substrate. The same correlation is found in islands with multiple layers.[13] One such example is shown in the image of Fig. 2(a) taken after deposition of 0.5 DL of Si at 420 °C. Island A has three different layers. The first layer is nucleated in the domain-boundary-free region of the substrate and consists entirely of 7×7 reconstructions. However, 5×5 and 2×1 reconstructions are found in the second and third layers, as shown in the atomically resolved images of Fig. 2(b). A careful inspection of the image in Fig. 2(b) shows that the formation of these metastable reconstructions is associated with domain boundaries in the layer below. As shown in Fig. 2(b), the portion of the second layer that has 5×5 reconstruction has grown on a region where there is a domain boundary in the first layer. Similarly, the 2×1 reconstruction in the third layer is associated with the domain boundary between the 7×7 and 5×5 reconstructions in the second layer. The experimental evidence we presented so far indicates that all islands with metastable structures are associated with domain boundaries in the underlying layer.

If the domain boundaries in the substrate are indeed responsible for the formation of 5×5 and 2×1 islands during homoepitaxial growth on Si(111), we should be able to change the population of islands with metastable reconstructions by manipulating the number of domain boundaries on the substrate. In one limit where there are no domain boundaries, the metastable structure should be absent from the islands, while in another limit where the substrate has many domain boundaries large numbers of islands with 5×5 or 2×1 reconstructions should be found. Experimentally, to obtain substrates with domain boundaries in the two extremes described above, special techniques in sample preparation have to be employed.

In Fig. 1(a), each single domain of 7×7 reconstruction in the substrate is bounded by two domain boundaries

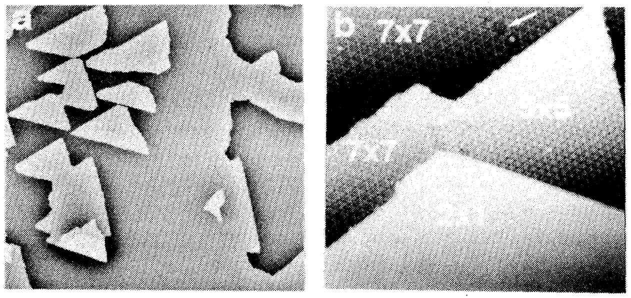

FIG. 2. (a) $750\times750\text{nm}^2$ image showing an island with three layers nucleated in a boundary-free region. (b) Atomically resolved image (75×75 nm^2, $-2-V$ bias) of the island in (e). The first layer has a 7×7 reconstruction while the second and third layers have 5×5 and 2×1 reconstructions, respectively. The 5×5 and 2×1 reconstructions are clearly correlated with the domain boundaries in the layer they grow upon. Arrows indicate the locations of domain boundaries.

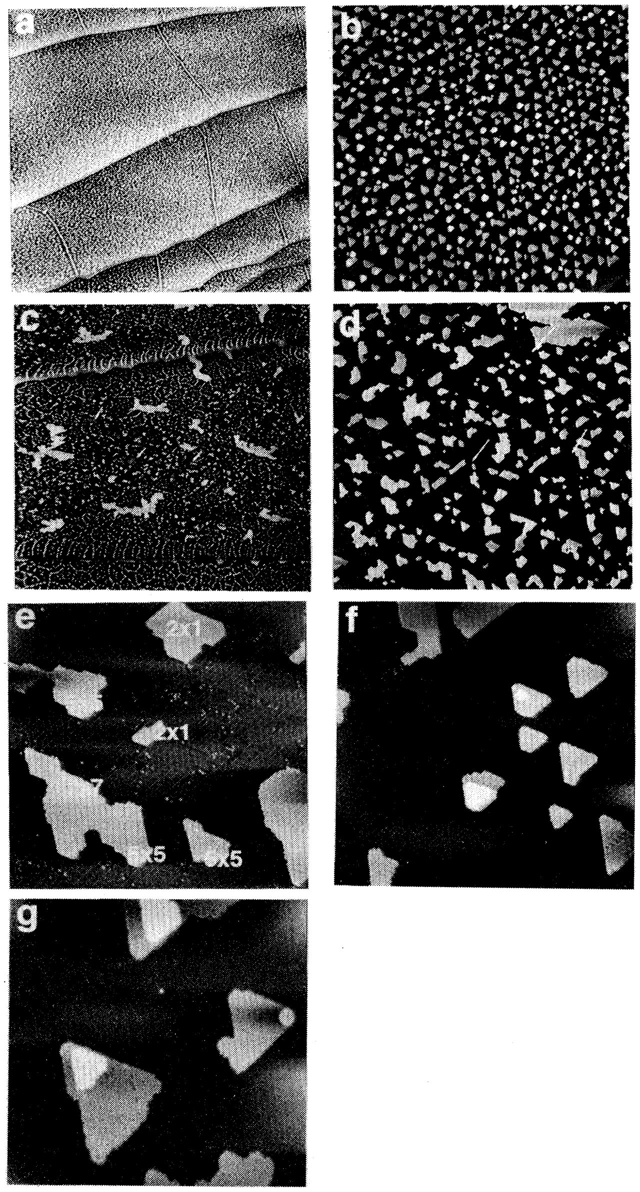

FIG. 3. (a) $3000\times3000\text{-nm}^2$ STM scan showing island formation on a substrate with a large 7×7 domain and few domain boundaries. (b) A closer view (750×750 nm^2) of the surface shown in (a). Except for some double-layer islands, all single-layer islands appear to have identical heights suggesting they have the same reconstruction. Atomically resolved images (not shown) reveal that they indeed all have a 7×7 reconstruction. (c) $3000\times3000\text{-nm}^2$ scan of island formation on a substrate with many domain boundaries. In contrast to the images in (a) and (b), there appears to be two different heights for the single-layer islands, suggesting different reconstructions in the islands. (d) $750\times750\text{-nm}^2$ STM scan showing 7×7 single domains and regions where many domain boundaries coexist on the same substrate. (e) $150\times150\text{-nm}^2$ image of a region with many domain boundaries showing many 5×5 and 2×1 islands. (f) $150\times150\text{-nm}^2$ image showing islands formed on the domain-boundary-free region. All have 7×7 reconstructions. (g) $75\times75\text{-nm}^2$ image of islands nucleated on a region free of domain boundaries. Even though the first layers of all islands have a 7×7 reconstruction, there are 5×5 reconstructions in the second layer.

and two step edges. As a result, the size of a 7×7 domain is $\sim L^2$, where L is the step separation. To reduce the number of domain boundaries, surfaces with large terraces between steps are needed. We generated terraces as large as 2000 nm from commercially available, flat Si(111) wafers with typical terrace sizes of 400 nm, using electromigration.[5–9] Substrates with few domain boundaries were then obtained by slowly cooling the sample from 900 °C to room temperature with a rate of 0.5 °C/s. Figure 3(a) shows a $3000\times3000\text{-nm}^2$ image of such a substrate after deposition of 0.3 ML of Si at 540 °C. Lines of islands in the image mark the location of domain boundaries. The number of domain boundaries per area is about four times less than that in the Fig. 1(a). Smaller-area scans (750×750 nm^2) of the surface in Fig. 3(b) show the most islands seem to have the same height, suggesting that they all have the same surface reconstruction. Indeed, among ~200 islands (nucleated on the domain-boundary-free region) we have examined with atomic resolution, all of them exhibit 7×7 reconstruction in the first layer and few have 5×5 reconstruction in the second layer. Some islands that have a brighter gray scale in Fig. 3(b) are double-layer islands.

To compare to the result on a substrate having few domain boundaries, we prepared a substrate with large number of domain boundaries by quenching the surface from 900 °C to room temperature with a rate of 100 °C/s after a large terrace size was obtained using electromigration. The surface morphology following deposition of, again, 0.3 ML at 540 °C is shown in Fig. 3(c). The large-size islands (with dimension > 300 nm) presented in the image are not due to the Si deposition; instead, they arise from the quick quench used to prepared the substrate. The detailed description of their formation and structures has been published previously.[5,6] The islands which were found following deposition of Si form the lines of islands at the step top and networks of islands at the step bottom, which again mark the location of domain boundaries in the near-step region. In the middle of the terrace, as we will show, the domain boundary density is much higher. In contrast to the islands on the domain-boundary-free substrate, many of the small islands grown in the middle of the terrace (indicated by arrows) have lower island height than the rest of the islands, suggesting a 2×1 reconstruction (on this scale, we cannot tell whether there are 5×5 islands because they have the same height as 7×7 islands). The smaller-area scans shown in Figs. 3(d)–3(g) confirm that indeed the formation of islands with metastable reconstructions has increased significantly. Figure 3(d) also reveals some other interesting aspects of this surface. There are two different types of regions coexisting on the substrate. Three triangular regions, each containing a single domain of 7×7 reconstruction in the substrate, can clearly be seen in Fig. 3(d). These 7×7 single domains were formed during the quench.[5,6] Outside of these triangular regions are regions with many domain boundaries, as evident from Fig. 2(d). The presence of the two types of regions provides an opportunity to further determine whether the 5×5 and 2×1 reconstructions are indeed caused by the domain boundaries in the substrate, because with the exception of the density of domain boundaries all other conditions, such as the growth temperature, deposition rate, and amount of impurities, are identical in the two regions.

Figure 3(e) shows an atomically resolved image of a region with a high density of domain boundaries. In addition to 7×7 islands, there are several islands with 5×5 or 2×1 reconstruction. In contrast, Fig. 3(f) shows an area inside one of the triangular regions. It shows that within this single domain of 7×7 reconstruction, the nucleated islands all have 7×7 reconstructions, including the second-layer islands. Two 2×1 islands can be seen at the edge of the region with high domain boundary density in the upper-left corner of the image. Figure 3(g) shows another area within a different triangular region. In this region, even though the first layer is entirely of 7×7 reconstruction, the second layers contain the 5×5 reconstruction again associated with domain boundaries on the underlying layer. Table I shows the population of 7×7, 5×5, and 2×1 islands, found in the two different types of regions. Within the 7×7 triangles, the islands nucleate on the domain-boundary-free substrate and thus have 7×7 reconstruction. Outside the 7×7 triangles, where there are high densities of domain boundaries, almost equal populations of 7×7, 5×5, and 2×1 islands are found.

DISCUSSION

The observation that islands nucleate at domain boundaries of the substrate is not terribly surprising. Because the bonding at domain boundaries represents slightly higher-energy configurations than the bonding in a defect-free region of the substrate, atoms which encounter a domain boundary during diffusion on a terrace may experience a stronger bond to the substrate at the domain boundary and a higher activation barrier to diffusion off of a domain-boundary site. Even a small increase in the residence time for adatoms at a domain boundary could significantly decrease the critical nucleus

TABLE I. Number of islands with different reconstructions found inside and outside triangular-shaped 7×7 single domains on the quenched sample of Fig. 3.

	Single-domain 7×7 regions		Regions of high domain density	
Reconstructions	First layer	Second layer	Population	%
7×7	15	3	46	34
5×5	0	2	46	34
2×1	0	0	44	32

needed for formation of an island via subsequent attachment of other randomly diffusing Si atoms.[14] Under these circumstances, we would expect to see homogeneous island formation only at distances greater than the diffusion length away from domain boundaries, consistent with our observations.

The surprising result from this study is that the formation of 5×5 and 2×1 reconstructions during homoepitaxial growth on Si(111) is facilitated in islands which have nucleated at domain boundaries in the substrate. The theoretical calculations of different reconstructions have shown that the energy difference between 7×7 and the two metastable reconstructions reported here, namely, 5×5 and 2×1, is on the order of a 10-meV/1×1 unit cell.[15–18] Thus small perturbations of the structure of a growing island may be sufficient to alter the energy balance favoring one of these three reconstructions over the other. There are two obvious mechanisms by which the presence of domain boundaries in the substrate could shift the energy balance in favor of one of the metastable reconstructions of Si(111). These are (1) edge effects and (2) density effects.

Edge effects arise because of the way in which the atoms at the edge of the islands are bound to the atoms in the substrate. When islands form on domain-boundary-free regions of a 7×7-reconstructed substrate, they ordinarily grow in a triangular shape[2] which allows the steps which comprise the island edges to be aligned in the favorable $[\bar{2}11]$ orientation.[19] There is a specific preferred registry of the 7×7 reconstruction across a step,[20] which presumably allows optimal bonding across the island edge. If the island lies on a domain boundary, then the steps which comprise the island edges cannot remain in registry on all three sides of the island without the introduction of either substantial stress or another domain boundary in the island. Thus the energy of a 7×7 island on a domain boundary will be increased, possibly enough to make the resulting energy comparable to that of the 5×5 or 2×1 reconstruction.[15] In both of these reconstructions, since the unit-cell spacing is different, it may also be possible to accommodate the underlying domain boundary while maintaining a favorable registry of all of the step edges with the substrate. In particular, this mechanism seems likely to play a role for the 2×1 reconstruction. Because it has twofold symmetry, rather than the threefold symmetry of the substrate, an island with 2×1 reconstruction can form with two edges running roughly parallel to a domain boundary as we (see Fig. 1) and others[4] observe. This configuration may allow optimization of the bonding across the edges of the island in spite of the disregistry with the underlying 7×7 reconstruction which is induced by the domain boundary.

The second mechanism which may play a strong role in stabilization of 5×5 and 2×1 islands at domain boundaries is a density effect. At a domain boundary, the translational disregistry of the reconstruction leads to a local change in the density of atoms. This change in density may be either a decrease or an increase. As an island grows on Si(111), the reconstruction of the substrate returns to the bulk 1×1 structure. However, near the domain boundary, the local density is perturbed so that the return to the 1×1 structure will require either a supply of additional atoms to the substrate (if the original domain wall was low density), or the release of additional atoms to the overlayer (low-density original domain wall). The domain wall thus effectively acts to change (locally) the thermodynamical potential conjugate to the atomic density, which is of course the chemical potential. Intuitively, we expect that variation in the local atomic density can affect the formation of the different reconstructions because they have different densities: the 7×7 reconstruction has a higher density of atoms than the bulk-terminated 1×1 structure, while the 5×5 and 2×1 reconstructions have the same densities as the bulk-terminated structure.[5,12,21,22] Vanderbilt has recently shown quantitatively how variations in the chemical potential can effect the relative stability of the different reconstructions of Si.[23] He modified his previous empirical model[15] for the energy ΔE_{DAS} of an $n\times n$ reconstruction in terms of the faulting energy, domain-wall formation energy, and corner hole formation energy to include the effect of a variable chemical potential. With this modification, the minimization of the free energy ΔE_{DAS}-$\mu\Delta N_{\mathrm{DAS}}$ (where ΔN_{DAS} is the excess density of atoms in the surface layer) is accomplished by replacing the previous wall and corner energies by effective energies including a contribution from the chemical potential. In this way, he has shown that variations in the chemical potential can stabilize the different reconstructions of Si(111) with respect to the 7×7 reconstruction.[23] Particularly, an increase in chemical potential stabilizes the higher-density reconstructions such as the 9×9, which are observed under conditions of supersaturation.[2,22] A decrease in chemical potential, as would occur under conditions of subsaturation, would stabilize the low-density 5×5 or 2×1 structures. Thus our observations of these low-density structures at domain walls (as well as previous observations of these structures during annealing of cleaved surfaces[12,21] may result from local conditions of Si atom density below the equilibrium density.

In conclusion, through examining homoepitaxial growth on Si(111) with a controlled density of domain boundaries, we have firmly established the correlation between the presence of domain boundaries in the substrate and the formation of islands with metastable 5×5 and 2×1 reconstructions. Based on this finding, the long observed presence of large percentages of metastable reconstruction on the Si(111) surfaces after high coverage growth is simply due to the large number of domain boundaries generated by the growth itself. Such a finding has a significant implication for epitaxial growth in general and Si growth in particular. The existence of domain boundaries encourages the formation of metastable structures as we have shown. In turn, the nucleation of metastable structures increases the number of domain boundaries. Together, they generate a process which accelerates the transition from the growth of ordered structures to the growth of disordered structures. Such a self-destructive mechanism could very well be responsible for the reported observation of the growth of amorphous layers beyond a certain thickness on Si(111), which has been attributed to the presence of impurities.[24]

ACKNOWLEDGMENTS

The authors would like to thank Norman C. Bartelt and Andres Fernandez for many useful discussions, and Elaine Fu for assistance in analyzing the data. This work was supported by the Office of Naval Research.

---

[1] M. H. V. Hoegen, J. Falta, and M. Henzler, Thin Solid Films **183**, 213 (1989).

[2] U. Kohler, J. E. Demuth, and R. J. Hamers, J. Vac. Sci. Technol. A **7**, 2860 (1989).

[3] Y.-N. Yang and E. D. Williams, Scanning Microscop. (to be published).

[4] T. Yokoyama, H. Tanaka, M. Itoh, T. Yokotsuka, and I. Sumita, Phys. Rev. B **49**, 5703 (1994).

[5] Y.-N. Yang and E. D. Williams, Phys. Rev. Lett. **72**, 1862 (1994).

[6] Y.-N. Yang and E. D. Williams, Scanning Microscop. (to be published).

[7] H. Tokumato and M. Iwatsuki, Jpn. J. Appl. Phys. **32**, 1368 (1993).

[8] A. V. Latyshev, A. L. Aseev, A. B. Krasilnikov, and S. I. Stenin, Surf. Sci. **213**, 157 (1989).

[9] Y. Homma, R. J. McClelland, and H. Hibino, Jpn. J. Appl. Phys. **29**, L2254 (1990).

[10] J. A. Stroscio, R. M. Feenstra, and A. P. Fein, Phys. Rev. Lett. **57**, 2579 (1986).

[11] R. M. Feenstra, J. A. Stroscio, and A. P. Fein, Surf. Sci. **181**, 295 (1987).

[12] R. M. Feenstra and M. A. Lutz, Surf. Sci. **243**, 151 (1991).

[13] We have found that islands nucleated in the region with no domain boundaries tend to have multiple layers, while islands on the domain boundaries are a single-layer high.

[14] J. A. Venables, Surf. Sci. **299/300**, 798 (1994).

[15] D. Vanderbilt, Phys. Rev. B **36**, 6209 (1987).

[16] K. D. Brommer, M. Needels, B. E. Larson, and J. D. Joannopoulos, Phys. Rev. Lett. **68**, 1355 (1992).

[17] I. Stich, M. C. Payne, R. D. King-Smith, J.-S. Lin, and L. J. Clarke, Phys. Rev. Lett. **68**, 1351 (1992).

[18] J. J. L. Mercer and M. Y. Chou, Phys. Rev. B **48**, 5374 (1993).

[19] E. D. Williams, R. J. Phaneuf, J. Wei, N. C. Bartelt, and T. L. Einstein, Surf. Sci. **294**, 219 (1993).

[20] J. L. Goldberg, X.-S. Wang, J. Wei, N.C. Bartelt, and E. D. Williams, J. Vac. Sci. Technol. A **9**, 1868 (1991).

[21] R. M. Feenstra and M. A. Lutz, Phys. Rev. B **42**, 5391 (1990).

[22] R. M. Feenstra and M. A. Lutz, in *The Structure of Surfaces III,* edited by S. Y. Tong, M. A. V. Hove, K. Takayanagi, and X. D. Xie (Springer-Verlag, Berlin, 1991), Vol. 24, p. 480.

[23] D. Vanderbilt, Scanning Microscop. (to be published).

[24] D. J. Eaglesham, H.-J. Gossman, and M. Cerullo, Phys. Rev. Lett. **65**, 1227 (1990).

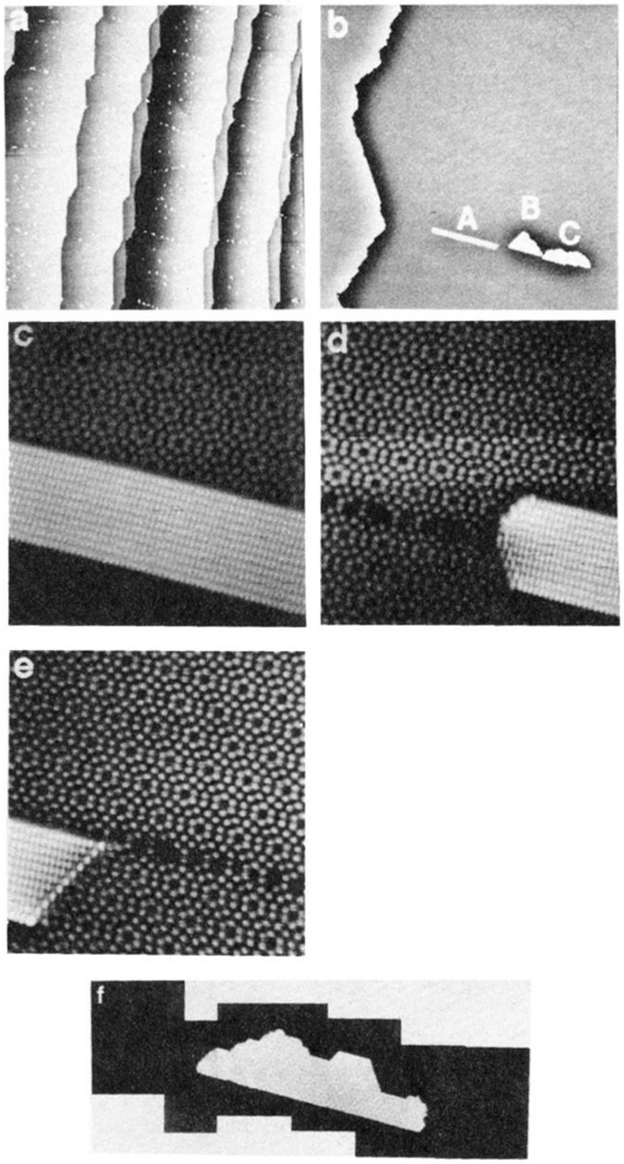

FIG. 1. (a) STM images of area 3000×3000 nm^2 after deposition of 0.03 DL of Si showing that islands nucleate preferentially at domain boundaries and randomly nucleate within single domains of 7×7 reconstruction. The sample temperature during deposition was 420 °C and the deposition rate was 0.003 DL/s. (b) Smaller-scale image (450×450 nm^2) showing three islands at a domain boundary. Island A has a 2×1 reconstruction, while islands B and C have 7×7 reconstructions. (c) Atomically resolved image of a middle section of island A showing the 2×1 reconstruction, and interfaces with the surrounding 7×7 reconstruction in the substrate. (d) and (e) Images of the two ends of the island A and the domain boundaries in the substrate. (f) A mosaic image of a 5×5 island at a domain boundary.

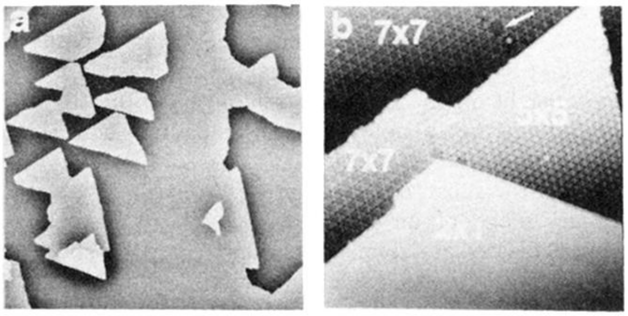

FIG. 2. (a) 750×750nm^2 image showing an island with three layers nucleated in a boundary-free region. (b) Atomically resolved image (75×75 nm^2, $-2-V$ bias) of the island in (e). The first layer has a 7×7 reconstruction while the second and third layers have 5×5 and 2×1 reconstructions, respectively. The 5×5 and 2×1 reconstructions are clearly correlated with the domain boundaries in the layer they grow upon. Arrows indicate the locations of domain boundaries.

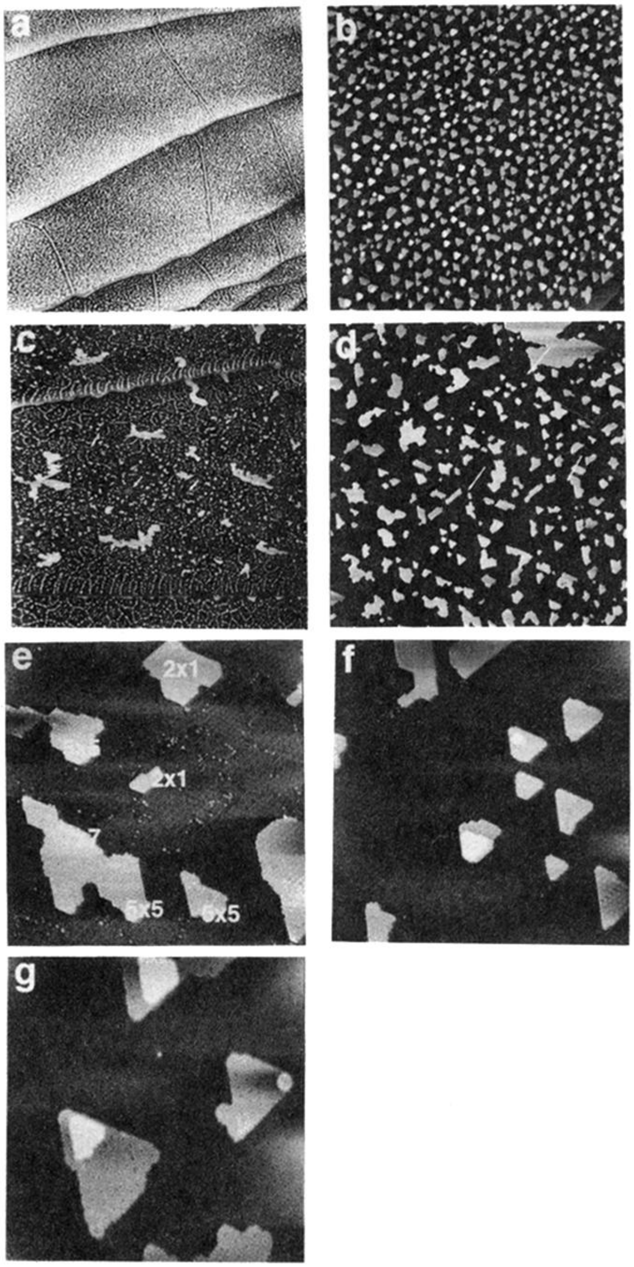

FIG. 3. (a) 3000×3000-nm^2 STM scan showing island formation on a substrate with a large 7×7 domain and few domain boundaries. (b) A closer view (750×750 nm^2) of the surface shown in (a). Except for some double-layer islands, all single-layer islands appear to have identical heights suggesting they have the same reconstruction. Atomically resolved images (not shown) reveal that they indeed all have a 7×7 reconstruction. (c) 3000×3000-nm^2 scan of island formation on a substrate with many domain boundaries. In contrast to the images in (a) and (b), there appears to be two different heights for the single-layer islands, suggesting different reconstructions in the islands. (d) 750×750-nm^2 STM scan showing 7×7 single domains and regions where many domain boundaries coexist on the same substrate. (e) 150×150-nm^2 image of a region with many domain boundaries showing many 5×5 and 2×1 islands. (f) 150×150-nm^2 image showing islands formed on the domain-boundary-free region. All have 7×7 reconstructions. (g) 75×75-nm^2 image of islands nucleated on a region free of domain boundaries. Even though the first layers of all islands have a 7×7 reconstruction, there are 5×5 reconstructions in the second layer.