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Initial stages of silicon molecular-beam epitaxy: Effects of surface reconstruction

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High-energy ion scattering and channeling and low-energy electron diffraction are used to investigate quantitatively the initial stages of interface formation (overlayer thickness up to ~10 Å) during Si molecular-beam epitaxy. Changes in the geometry of the Si substrate surface (i.e., reordering) and of the Si overlayer are measured as a function of Si coverage, deposition temperature, and substrate reconstruction. It is found that room-temperature deposition reorders the Si(100)-2×1 substrate but not the Si(111)-7×7. This difference is discussed in terms of structural models for these surfaces. On both surfaces, however, deposition at 300 K results in a highly imperfect overlayer. To obtain high-quality growth, a deposition temperature of ~790 K is needed for Si(111)-7×7 and of ~570 K for Si(100)-2×1. The implications of these results with respect to molecular-beam epitaxy are discussed.

I. INTRODUCTION

Molecular-beam epitaxy (MBE) refers to the controlled deposition of material onto an atomically clean solid surface. Under the proper conditions of substrate temperature, deposition rate, and lattice match between the overlayer and substrate, a uniform, epitaxial layer with a low defect density is achievable. In most cases of small lattice mismatch, and always for the case of homoepitaxy, the crystal structure of the overlayer is pseudomorphic with respect to the bulk substrate. The atoms in the surface monolayer(s) of a clean material are usually not in their "bulklike" sites but reconstructed. The MBE process on the other hand results in an interface with atoms at bulklike sites. This then naturally raises the question of "reordering," and the general role of reconstruction, in epitaxial growth. In this paper we report measurements of this reordering process as a function of crystal orientation and substrate temperature for the technologically important case of Si homoepitaxy.

MBE has had its largest use and greatest success in semiconductor applications. It is this class of materials for which questions of surface reconstruction are most relevant, as many semiconductor surfaces exhibit strong reconstruction effects. In the case of Si(100) and Si(111), the common surface reconstructions are known to exhibit large atomic displacements and extend three to four monolayers (ML) below the surface.[1-3]

Recently, we reported[4,5] results on the changes in surface reconstruction associated with deposition of up to 10 Å of Ge on Si(100)-2×1 and Si(111)-7×7. Our findings indicated that the Si reordering is a temperature-activated, chemisorption-induced process, sensitive to the details of the substrate reconstruction. We found that the Si(100) surface reorders at temperatures as low as 300 K while the Si(111)-7×7 surface reordering requires temperatures well above room temperature. In both cases, at the appropriate temperature, the reordering was observed to obey a monolayer-by-monolayer dependence, that is one monolayer of Ge deposition induced one monolayer of Si to reorder. For both surfaces and at all growth temperatures the atoms in the resulting Ge layer had significant displacements from bulklike sites. In the case of the Ge/Si system it is probable that the large lattice mismatch (~4.2%) plays a significant role in the determination of epitaxial growth and interface structure. For example, the large strain energy associated with the mismatched system represents a possible driving force for interdiffusion at the solid-state interface. We were thus motivated to study the apparently simpler system of Si homoepitaxy. Our findings indicate that the substrate reordering process is very similar to that observed for the GeSi system, as expected, but the epitaxial growth of the overlayer is quite different.

The main tools used in our study are the surface-sensitive probes of low-energy electron diffraction (LEED) and high-energy ion scattering [Rutherford backscattering (RBS)/channeling]. The latter is a mass-dispersive crystallography[6] particularly useful for studies of heteroepitaxy, as we have demonstrated in the investigation of the GeSi system cited above. Even in case of homoepitaxy, however, ion scattering provides a quantitative measure of the total surface and subsurface reconstruction which is not readily available by other techniques. LEED is, of course, an invaluable surface-structure tool for revealing the surface long-range order. In an early and thoughtful study, Jona[7] has carried out similar Si homoepitaxy experiments using LEED in a qualitative and semiquantitative mode. While our experimental LEED results are in qualitative agreement with this earlier work, the supplementary information based on the ion scattering experiments and the experience with the Ge/Si systems leads us to some new interpretations of the growth process.

II. EXPERIMENTAL

The present study was performed in a standard ultrahigh vacuum system (base pressure 5×10^{-9} Pa) equipped with Auger spectroscopy, low-energy electron diffraction, sample sputtering and heating facilities, and a

Knudsen-cell-type oven. This system is coupled to a Van de Graaff accelerator for ion scattering surface analysis. Si(111) and Si(100) samples (polished wafers cut to within 0.5° of the surface plane), cleaned by sputtering at room temperature and annealing to 1200 K displayed a sharp 7×7 and 2×1 LEED pattern, respectively, an Auger spectrum indicating a clean surface and ion scattering surface-peak (SP) intensities in good agreement with previous measurements.[2–4] Quantitative determinations of SP intensities and coverages were made by employing a Bi-implanted Si standard of known areal density. Deposition was carried out on cleaned Si substrates held at a particular temperature at rates of ~ 0.1 ML/min. [In the following we define 1 ML as the number of sites at a Si surface, 7.830×10^{14} cm^{-2} for Si(111) and 6.782×10^{14} cm^{-2} for Si(100), respectively.] Although deposition was carried out at different temperatures, all measurements were performed at 300 K. During deposition the background pressure never exceeded 8×10^{-8} Pa. Auger-electron spectroscopy (AES) indicated only slight contamination ($\lesssim 0.01$ ML) with carbon and oxygen for growth temperatures below 570 K, and none at 790 K.

An important advantage of ion scattering is the capability of quantitative coverage measurements for deposition of material onto a substrate. Accurate coverage measurements are essential for the interpretation of epitaxial growth studies. However, standard RBS relies on the fact that substrate and overlayer have different masses; otherwise a separation of substrate and overlayer in the energy spectrum of the scattered projectiles is not possible. To circumvent this inherent difficulty for homoepitaxial systems with overlayer thicknesses in the few monolayer range, we arranged a carbon block ~ 5 mm away from the Si sample and obtained the coverage from a measurement of the Si-covered carbon. Each time the Si sample was prepared as described above, we also sputtered the carbon block to remove the Si deposited during the preceding run. This procedure assumes that (1) the sticking coefficient of Si on carbon is identical to Si on Si, and (2) that the impinging Si flux is sufficiently homogeneous over the distance between Si sample and carbon block. The internal consistency of our results demonstrates that this is the case. Further, assumption (1) is not needed for deposition beyond 1 ML as then Si is deposited on a Si-coated carbon block. Nevertheless this procedure of coverage measurements might introduce a systematic error beyond that normally quoted for RBS; a conservative estimate of the maximum total uncertainty of absolute coverage measurements is ±10%.

III. RESULTS

The main quantity obtained in our measurements is the total Si surface-peak intensity as a function of Si coverage in the range from 0–7 ML. As discussed above separation of a few ML thick Si overlayer from the Si substrate is not possible in an RBS spectrum; therefore only the total (overlayer plus substrate) SP is accessible. Unless specifically stated we will subsequently refer to this combined quantity simply as the surface peak. The interpretation of the SP dependence on coverage and growth parameters is aided by the evolution of the LEED pattern, which we will also discuss.

Depending on the particular growth mode present, the SP intensity will show a particular dependence on the Si coverage. We schematically illustrate this dependence for some simple growth models in Fig. 1. The various panels show the SP intensitites of a hypothetical, simple cubic crystal as a function of coverage for deposition of addi-

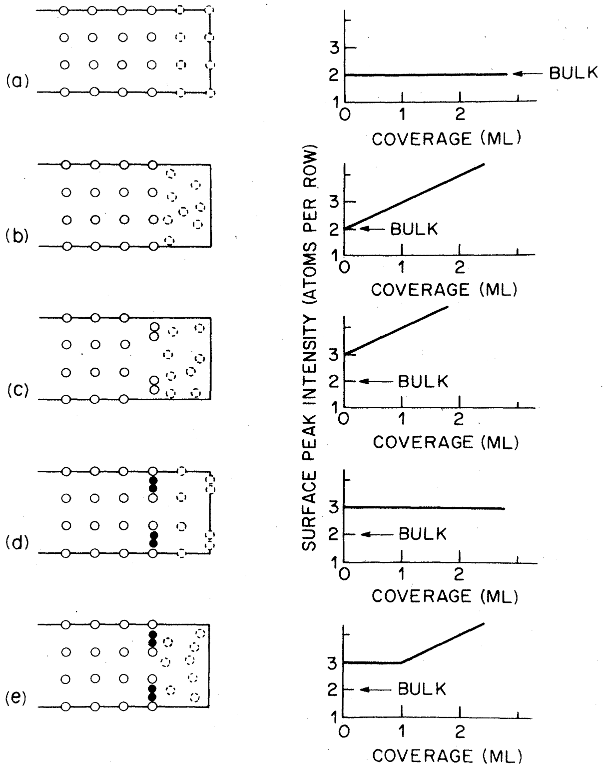

FIG. 1. Schematic of different overlayer structures and their expected surface peak (SP) dependence as a function of coverage for the case of homoepitaxy. (a) Epitaxial growth on a bulklike structure—the SP is given by the "bulklike" value and constant as a function of coverage. (b) A disordered layer on top of a "bulklike" crystal surface—the SP has a "bulklike" value for zero coverage and increases linearly with increasing coverage. (c) A disordered layer on top of a reconstructed surface—the SP has a zero coverage value corresponding to the "bulklike" structure plus the number of reconstructed layers; the SP increases linearly with coverage for the "disordered" layer growth. (d) Epitaxial growth on an originally reconstructed surface, the reconstruction is maintained at the vacuum-epilayer interfaces—the SP value at zero coverage corresponds to the reconstructed surface and remains constant as a function of epitaxial growth. (The solid dots indicate the original positions of atoms in the substrate surface.) (e) A disordered layer on an originally reconstructed surface which has reordered as a result of the overlayer—the SP at zero coverage corresponds to the reconstructed surface value, and remains constant as a function of coverage as one monolayer worth of disordered atoms "replaces" one monolayer of reconstructed atoms. The value remains constant to a coverage corresponding to the total number of reconstructed layers and then increases linearly with coverage as the disordered layer grows.

tional substrate material assuming different growth models. Normal incidence of the ion beam is assumed. The SP intensities are usually expressed as the number of atoms per row visible to the beam;[6] in this hypothetical case 1 atom per row corresponds to 1 ML. Circles with dashed circumference symbolize deposited atoms, those with solid circumference substrate atoms. Figure 1(a) shows perfect epitaxial growth on an unreconstructed substrate. The initial, zero coverage value of the SP corresponds to that expected from an ideal single crystal; it is usually greater than unity due to finite thermal vibrations exposing the second and deeper atoms to a certain degree. Here we arbitrarily assume a clean surface value of 2 atoms per row. If the deposited material simply continues the substrate growth, as assumed in Fig. 1(a), the measured SP remains at a constant value. This is contrasted with the type of growth in Fig. 1(b), where the overlayer is in a disordered state. Under these conditions the overlayer does not shadow the substrate from the incident beam. The scattering intensity from the surface is then proportional to the number of ML in the disordered overlayer plus the (constant) contribution from the substrate surface peak. The total SP intensity therefore rises linearly with coverage; the slope of the straight line is precisely 1 atom per row per ML.

Figure 1(c) illustrates the expected result for cases similar to that of 1(a) and 1(b) but on a reconstructed substrate. Here the initial value of the SP intensity is higher than that expected for the bulk structure due to surface reconstruction. We arbitrarily assume that only the first-layer atoms are displaced preventing shadowing of the second or underlying layers and giving rise to an enhancement of the SP intensity by 1 atom per row. If subsequent deposition results in a disordered layer with no change in the substrate structure, the scattering intensity simply increases linearly with coverage [as in Fig. 1(b) but displaced along the vertical axis by the number of reconstructed substrate layers].

Under the proper conditions we can expect a high-quality crystalline growth of the overlayer where the reconstruction "stays" constantly at the vacuum-solid interface of the growing crystal, the next-to-last layer constantly reordering. For this case the SP is a constant as a function of coverage with an absolute value corresponding to the reconstructed surface [Fig. 1(d)]. Finally, we can imagine a growth mode suggested by the Ge/Si results: namely a reordering of the substrate (each monolayer deposited reorders one monolayer of reconstruction) but a

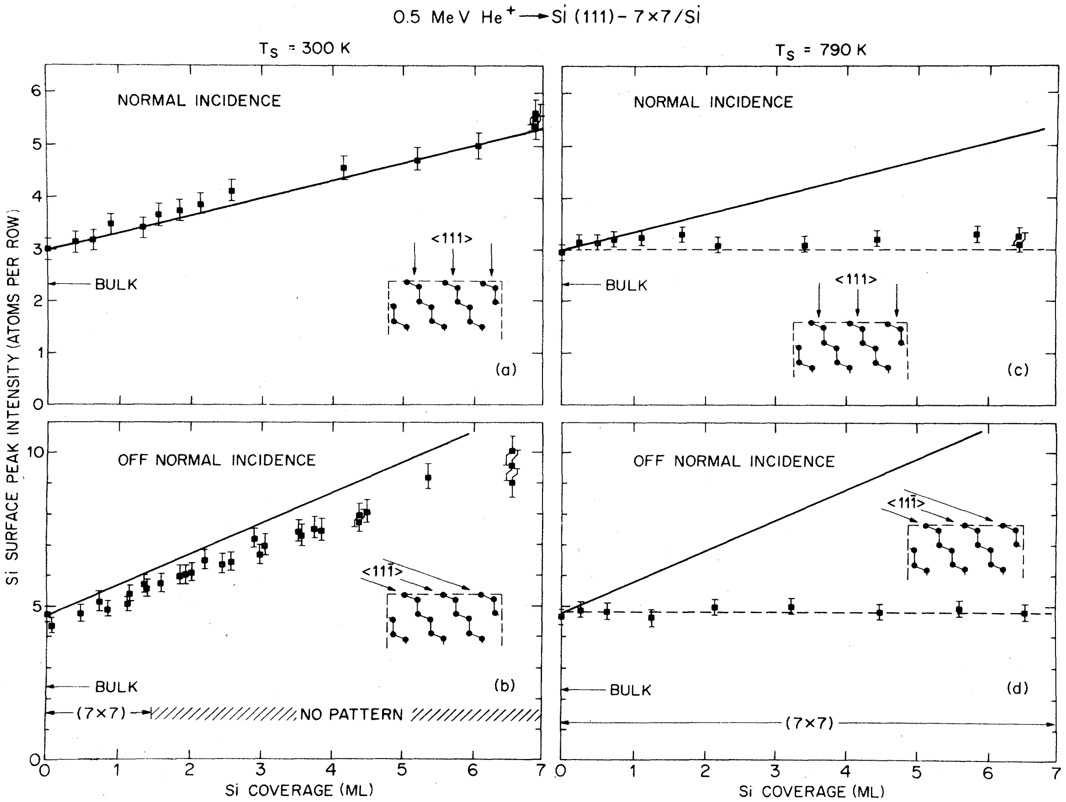

FIG. 2. Si SP (using 0.5-MeV He$^+$) as a function of Si coverage on Si(111)-7×7 for (a) deposition at 300 K and measurement along the ⟨111⟩ normal direction (1 atom per row = 3 ML), (b) deposition at 300 K and SP measured along the ⟨11$\bar{1}$⟩ off-normal direction (1 atom per row = 1 ML), (c) deposition at 790 K and measured along the ⟨111⟩ normal direction, and (d) deposition at 790 K and measured along the ⟨11$\bar{1}$⟩ off-normal direction. All SP measurements are at room temperature. In each figure the arrow at 2.3 atoms per row indicates the bulklike value. The evolution of the LEED pattern as a function of coverage is indicated. The solid line represents the expected dependence for growth of a disordered layer on a reconstructed surface [see Fig. 1(c)]. Insets schematically show the scattering geometry (side view).

disordered overlayer. The SP dependence for this situation is shown in Fig. 1(e). A monolayer of displaced overlayer is deposited allowing a monolayer of reconstructed substrate to reorder, keeping the total SP at a constant value. The surface peak remains constant until substrate reordering is complete (1 ML in this hypothetical case). After this point the SP intensity increases linearly with coverage as in Fig. 1(c). Note that for this mode we cannot easily distinguish if the first layer goes down ordered but reconstructed, or disordered.

Experimental results are shown in Figs. 2(a)—2(d) for homoepitaxy on the Si(111)-7$\times$7 surface and in Figs. 3(a) and 3(b) for the Si(100)-2$\times$1 surface. Measurements on the (111) surface are for the normal direction, $\langle 111\rangle$, where 1 atom per row corresponds to three monolayers and along the $\langle 11\bar{1}\rangle$ direction (70.8° away from the surface normal), where 1 atom per row corresponds to one monolayer. In the case of the (100) surface, measurements are made in the $\langle \bar{1}\bar{1}1\rangle$ direction (at 54.7° to the surface normal) to enhance the surface sensitivity. Here 1 atom per row corresponds to two monolayers. Since all the measurements are along $\langle 111\rangle$-type directions all the plots have the same bulklike value of 2.3 atoms per row, indicated by the short arrow. Also indicated in Figs. 2(b), 2(d), and Fig. 3 is a description of the LEED pattern as a function of coverage.

Figures 2(a)-2(d) show the Si SP intensity as a function of Si coverage for deposition on Si(111)-7$\times$7 at 300 K and 790 K. For room temperature deposition [Figs. 2(a) and 2(b)] the growth pattern is like that schematically shown in Fig. 1(c), a displaced overlayer on top of a reconstructed substrate, where the reconstruction appears unaffected by the overlayer. The expected dependence of the total SP intensity on Si coverage, taking into account the proper conversion from atoms per row to ML, is then given by the solid lines in Fig. 2(a) (normal incidence) and Fig. 2(b) (off-normal $\langle 11\bar{1}\rangle$ incidence). While the agreement for normal incidence, where channeling is only sensitive to lateral displacements, is excellent, the off-normal incidence data in Fig. 2(b) shows a small but reproducible difference from the expected dependence. Although the discrepancy is within our limit of uncertainty for absolute coverage determination, it might be associated with a very local short-range ordering, as in bilayer growth, affecting only normal displacements. Nevertheless the dominating effect for deposition of Si on Si(111)-7$\times$7 at 300 K is growth of a disordered layer on top of an inert reconstructed substrate surface.

We note that these results are inconsistent with a simple relaxation model of the 7$\times$7 surface.[3] In this case one might expect a large change in surface relaxation upon deposition of Si. Such a model was originally proposed[3] on the basis of detailed SP measurements as a function of energy and incident angle to account for the apparent small lateral, but large normal displacements of the Si(111)-7$\times$7 reconstruction. However, more recent analyses show that these data are also consistent with a surface stacking fault,[8] which would not necessarily be altered by the Si overlayer.

In contrast to the 300 K data, deposition at high temperature (790 K) is precisely that expected for semiconductor epitaxy [Fig. 1(d)]. The value of the surface peak remains constant with Si deposition and the LEED pattern shows consistently a high-quality 7$\times$7 pattern [Fig. 2(d)]. Clearly this is an adequate temperature (at this deposition rate) for epitaxial growth.

Results for deposition of Si on Si(100)-2$\times$1 are shown in Figs. 3(a) and 3(b). For deposition at 300 K [Fig. 3(a)] the growth pattern is similar to that schematically described in Fig. 1(e). The surface-peak value remains constant up to a coverage of ~3 ML and then increases linearly with further coverage. Note that three monolayers is just the observed excess of the zero coverage surface peak over that of the expected bulk value, i.e. ion scattering observes three monolayers of atoms to be displaced more than ~0.1 Å. Thus initial growth is consistent with either good epitaxy [Fig. 1(d)] or a reordering of the substrate layers by a disordered (displaced) overlayer [Fig. 1(e)]. We can rule out the former case since (1) the LEED pattern does not represent a sharp 2$\times$1 beyond 1 ML coverage and (2) the SP intensity does not remain

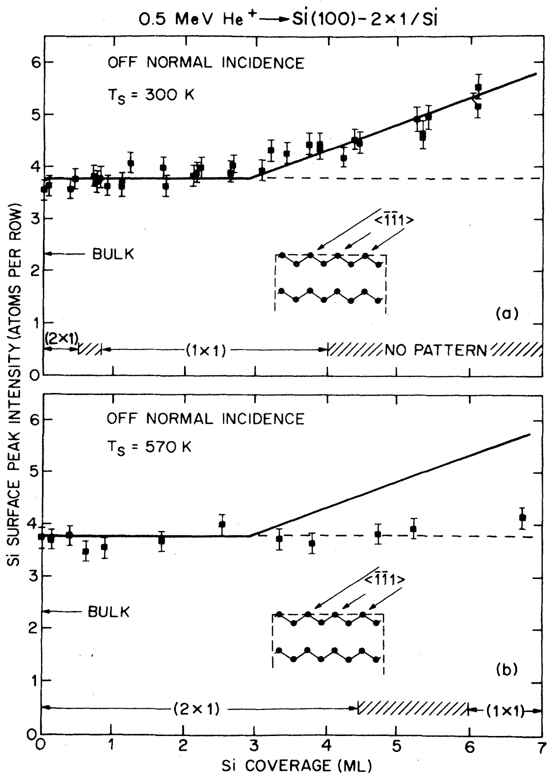

FIG. 3. Si SP (using 0.5-MeV He$^+$) as a function of Si coverage on Si(100)-2$\times$1. (a) Deposition at 300 K and measurement along the $\langle \bar{1}\bar{1}1\rangle$ off-normal direction. (For this direction 1 atom per row = 2 ML.) (b) Deposition at 570 K and measurement along the $\langle \bar{1}\bar{1}1\rangle$ direction. All SP measurements are at room temperature. In each figure the arrow at 2.3 atoms per row indicates the bulklike value. The evolution of the LEED pattern as a function of coverage is indicated. The solid line represents the expected dependence for growth of a disordered layer on a surface which reorders as a result of the overlayer [see Fig. 1(e)]. Insets schematically show the scattering geometry (side view).

constant beyond 3 ML but increases linearly with coverage. The rate of increase is precisely given by 0.5 atoms per row per ML, as expected for growth of an overlayer containing many large displacements (solid line). Up to ~4 ML some degree of long-range order might be preserved as a (1×1) pattern is observed to coverages of ~4 ML. [Compare this situation of Figs. 2(a) and 2(b) where the 7×7 pattern is not visible beyond one layer coverage.] This does not constitute a contradiction to the ion scattering results: LEED is mainly sensitive to the first layer and its long-range order. For the ion beam, on the other hand, any layer containing atoms displaced from bulklike sites more than ~0.1 Å will appear disordered, regardless of whether these displacements form a regular array, i.e, show some long-range order, or not. Although a regular array of displacements in a layer would be compatible with our channeling results, the displacements would have to be different from monolayer to monolayer; otherwise shadowing in the overlayer itself would reduce the increase in SP intensity as a function of coverage below 0.5 atoms per row per ML. In other words, we can clearly exclude that Si grows on Si(100)-2×1 at 300 K in an ideal, bulklike geometry, as suggested by Jona[7] and de Jong *et al.*[9]

Figure 3(b) shows (100) growth at 570 K. The initial stages of growth (up to ~4 ML) are precisely as expected for high-quality epitaxy although some indication of disorder is observed in the six—seven monolayer range. Still higher temperature deposition produces LEED patterns and surface-peak intensities consistent with high-quality epilayers for very thick films.

Finally we note that the above discussed dependencies of the total SP intensity on Si coverage for room-temperature deposition constitute a sensitive consistency check on our assertion (see Sec. II) that the Si coverage as measured on the carbon block is identical to the coverage on the Si substrate. We have pointed out above that at 300 K the overlayer contains large lateral displacements, i.e., appears amorphous to the ion beam. If the substrate contribution to the SP intensity stays constant, as is the case at 300 K for Si(111)-7×7 over the whole investigated coverage range, and for Si(100)-2×1 beyond a coverage of 3 ML, then the deposition of Si will lead to a linear increase in total SP intensity. Its slope is precisely 1 ML of SP increase for every ML Si deposited [solid lines in Figs. 2(a) and 3(a)]. If the sticking coefficients of Si on C would significantly differ from Si on Si the experimentally observed slope would show a significant deviation from unity. This, however, is not observed; the experimental data precisely follow a unity slope.

IV. DISCUSSION AND CONCLUSION

It is clear from these results that the (111) and (100) Si surfaces have different temperature dependencies for homoepitaxy. This fact has already been observed by Jona[7] and appears to be an empirical finding by the Si MBE community. Here we have shown that at least one factor in this difference is the nature of the reconstruction of the substrate surface. From the behavior of the total Si SP intensity as a function of coverage for different temperatures we can also deduce epitaxial temperatures: ~790 K for growth on Si(111)-7×7 and ~570 K for growth on Si(100)-2×1. This is in reasonable agreement with other work,[7,9,10] where the quality of the LEED pattern after deposition was used to determine an epitaxial temperature.

Our results are consistent with the previously reported[4,5] case of Ge deposition on Si. For both, deposition of Ge and Si, the Si(100) reconstruction is reordered for room-temperature deposition, while high-temperature deposition is required to relieve the Si(111)-7×7 reconstruction. For the case of Ge deposition, it was found that the epilayer showed no evidence of either short- or long-range order. Building on the analogy, we can infer that the Si(100) epilayer (for 300 K deposition) is also disordered and the major effect of Si deposition on the (100) surface is to reorder the substrate reconstruction.

Not only is there an analogy between the behavior of Si/Si reordering and Ge/Si reordering but also between the surface reordering behavior under atomic hydrogen adsorption. Briefly, the Si(111)-7×7 shows only a diminution of the LEED pattern upon hydrogen adsorption at room temperature,[11] while the Si(100) reconstruction changes from 2×1 to 1×1.[12,13] The substrate SP intensity shows no change in the case of Si(111).[14] For Si(100) it is reduced, although, unlike the case of Ge or Si deposition at room temperature, it does not reach the bulk value. However, recent work[15] indicates that at the H-saturated Si(100) surface only about half of the H is bonded as dihydride, which would be expected to lead to a reordered substrate, whereas the rest form monohydrides that preserve the dimers and the displacements of substrate atoms from bulklike sites.

This reordering behavior is qualitatively consistent with our understanding of the nature of the reconstruction in these two surfaces. An extensive body of evidence indicates that the Si(100)-2×1 surface consists of asymmetric dimers[1,16–19]—a smooth or atomically complete reconstruction involving Si pairing that "ties-up" dangling bonds. The reordering apparently occurs as a result of the deposited atoms breaking dimer bonds and allowing the substrate to reorder.

The understanding of the 7×7 surface is not as definitive but current models[20–26] support a rough or atomically incomplete reconstruction, possibly involving a stacking fault structure with further atomic rearrangements.[8] The reordering in this case would require substantial atomic motion (not just bond breaking) which cannot take place at room temperature, given available estimates for Si on Si surface diffusion constants.[27–29] Hence, the reordering can only occur at high temperature.

This reasoning suggests that surfaces with structures involving a minimum of roughness are good candidates for lower-temperature MBE growth. This is particularly applicable in the case of heteroepitaxy where interdiffusion at the interface is of concern. Possibly it is the same reconstruction argument which makes GaAs(100) such a favorable surface for MBE growth, since this surface is also modeled as a simple dimer reconstruction.

Finally, we note that surface reordering is only one mechanism in the MBE process. Clearly surface diffusivity and growth rate must be important factors in producing uniform layered structure. Indeed this must be the dominant factor as we have shown that reordering can take place at room temperature in Si(100) yet it is apparently not possible to grow an epitaxial layer at 300 K. Nevertheless, we have demonstrated that the reordering is temperature dependent and surface specific; it may be a determining factor in choosing a suitable candidate for molecular-beam epitaxy.

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[1] J. A. Appelbaum and D. P. Hamann, Surf. Sci. **74**, 21 (1978).

[2] L. C. Feldman, P. J. Silverman, and I. Stensgaard, Nucl. Instrum. Methods **168**, 589 (1980).

[3] R. J. Culbertson, L. C. Feldman, and P. J. Silverman, Phys. Rev. Lett. **45**, 2043 (1980).

[4] H.-J. Gossmann, L. C. Feldman, and W. M. Gibson, Phys. Rev. Lett. **53**, 294 (1984).

[5] H.-J. Gossmann, L. C. Feldman, and W. M. Gibson, Surf. Sci. (to be published).

[6] L. C. Feldman, J. W. Mayer, and S. T. Picraux, *Materials Analysis by Ion Channeling* (Academic, New York, 1982).

[7] F. Jona, in *Proceedings of the 13th Sagamore Army Materials Research Conference, Raquette Lake, N.Y., Aug. 23—26, 1966,* edited by J. J. Burke, N. L. Reed, and V. Weiss (Syracuse University Press, Syracuse, N.Y., 1967), p. 399.

[8] P. A. Bennett, L. C. Feldman, Y. Kuk, E. G. McRae, and J. E. Rowe, Phys. Rev. B **28**, 3656 (1983).

[9] T. de Jong, W. R. S. Douma, L. Smit, V. V. Korablen, and F. W. Saris, J. Vac. Sci. Technol. **B 1**, 888 (1983).

[10] K. D. Gronwald and M. Henzler, Surf. Sci. **117**, 180 (1982).

[11] E. G. McRae and C. W. Caldwell, Phys. Rev. Lett. **46**, 1632 (1981).

[12] T. Sakurai and H. D. Hagstrom, Phys. Rev. B **14**, 1593 (1976).

[13] S. J. White and D. P. Woodruff, Surf. Sci. **63**, 254 (1977).

[14] R. J. Culbertson, L. C. Feldman, and P. J. Silverman, J. Vac. Sci. Technol. **20**, 868 (1982).

[15] Y. J. Chabal and Krishnan Raghavachari, Phys. Rev. Lett. **54**, 1055 (1985).

[16] R. E. Schlier and H. F. Farnsworth, J. Chem. Phys. **30**, 917 (1959).

[17] D. J. Chadi, Phys. Rev. Lett. **43**, 43 (1979).

[18] M. Aono, Y. Hou, C. Oshima, and Y. Ishizawa, Phys. Rev. Lett. **49**, 567 (1982).

[19] R. M. Tromp, R. G. Smeenk, F. W. Saris, and D. J. Chadi, Surf. Sci. **133**, 137 (1983).

[20] E. G. McRae, Surf. Sci. **124**, 106 (1983).

[21] E. G. McRae, Phys. Rev. B **28**, 2305 (1983).

[22] G. Binnig, H. Rohrer, C. H. Gerber, and E. Weibel, Phys. Rev. Lett. **50**, 120 (1983).

[23] Y. J. Chabal, Phys. Rev. Lett. **50**, 1850 (1983).

[24] E. Conrad and M. B. Webb, Surf. Sci. **129**, 37 (1983).

[25] F. J. Himpsel, Phys. Rev. B **27**, 7782 (1983).

[26] M. Aono, R. Souda, C. Oshima, and Y. Ishizawa, Phys. Rev. Lett. **51**, 801 (1983).

[27] W. K. Burton, N. Cabrera and F. L. Frank, Philos. Trans. Soc. London, Ser. A **243**, 299 (1951).

[28] E. Kasper, Appl. Phys. **A28**, 129 (1982).

[29] Y. J. Chabal, J. E. Rowe, and S. B. Christman, Phys. Rev. B **24**, 3303 (1981).