# Reordering of Reconstructed Si Surfaces upon Ge Deposition at Room Temperature

H.-J. Gossmann
*State University of New York at Albany, Albany, New York 12222, and AT&T Bell Laboratories, Murray Hill, New Jersey 07974*

and

L. C. Feldman
*AT&T Bell Laboratories, Murray Hill, New Jersey 07974*

and

W. M. Gibson
*Department of Physics, State University of New York at Albany, Albany, New York 12222*
(Received 2 April 1984)

The behavior of the Si(111)-(7×7) and the Si(100)-(2×1) surfaces upon room-temperature deposition of Ge is investigated with Auger-electron spectroscopy, low-energy electron diffraction, and Rutherford backscattering channeling techniques. The Ge overlayers form a sharp, but highly disordered, interface with no indication of island formation. It is found that the Ge relieves the reconstruction of the Si(100)-(2×1) surface but not of the Si(111)-(7×7) surface.

PACS numbers: 68.20.+t, 61.80.Mk, 68.55.+b

The first stages of interface formation are of increasing interest in solid state physics from both a fundamental and a technological point of view. In the case of semiconductors, growth of thin, layered, epitaxial structures often takes place on a reconstructed surface whose atomic arrangements differ from those of the bulk substrate. As growth proceeds beyond one layer the reconstructed surface-vacuum interface becomes a solid-solid interface with the possibility of new atomic positions or even reordering.

We have studied this possible reordering for Ge deposition on Si(111)-(7×7) and Si(100)-(2×1) surfaces. An extensive body of data as a function of temperature and crystal orientation shows that both surfaces reorder for high-temperature ($\gtrsim 300\,\mathrm{C}°$) Ge deposition. However, for room-temperature growth we find a surprising difference in this reordering between the Si(111)-(7×7) and the Si(100)-(2×1) reconstruction. This is the first observation of this phenomenon, which provides important clues as to the nature of these extensively studied surfaces and the influence of surface reconstruction on epitaxy.

The present study was performed in a standard ultrahigh-vacuum system equipped with Auger spectroscopy, low-energy electron diffraction (LEED), sample sputtering and heating facilities, and a Knudsen-cell-type Ge oven. This system was coupled to a van de Graaff accelerator for ion-scattering surface analysis.[1,2] Si(111) and Si(100) samples, cleaned by sputtering at room temperature and annealing to 930 °C, displayed sharp (7×7) and (2×1) patterns, respectively, an Auger spectrum indicating a clean surface, and ion-scattering surface peak (SP) intensities in good agreement with previous measurements.[3,4] Ge deposition was carried out on cleaned Si substrates held at room-temperature at rates of $\approx 0.1$ ML/min. [In the following we define 1 ML (monolayer) as the number of sites at a Si layer, $7.830\times 10^{14}\ \mathrm{cm}^{-2}$ for Si(111) and $6.782\times 10^{14}\ \mathrm{cm}^{-2}$ for Si(100).] The growth mode of Ge was determined by measuring the intensity of the 92-eV Si($LVV$) Auger line as a function of Ge coverage. For Si(100)-(2×1) as well as Si(111)-(7×7)[5] it exhibits the exponential-type decay characteristic for simple growth without islanding or indiffusion.

The primary interest in this experiment is the behavior of the reconstructed Si surface upon Ge deposition. Ion scattering provides a convenient way of studying this phenomena as it is a mass-dispersive crystallography applicable to surface and near-surface regions of solids. Two quantities are obtained from the ion-scattering experiments[1,2]: (1) The Ge minimum yield as a function of adsorbate coverage, which yields information about the atomic ordering in the overlayer. For the first few layers this property is also accessible by observation of the LEED pattern. (2) The substrate surface peak as a function of adsorbate coverage which is a measure of either the reordering of a reconstructed surface and/or the shadowing of the substrate by the epitaxial overlayer.


©1984 The American Physical Society

We will show subsequently that in the work presented here epitaxial shadowing of the substrate by the Ge overlayer can be excluded. Any change in the Si SP intensity is therefore directly related to a change in reconstruction. As indicated in the bottom part of Fig. 1(c) the $(7\times7)$ pattern slowly fades away with increasing coverage until beyond $\approx 1.3$ ML no pattern is observable. This evidence of a disordered overlayer is further supported by the constant value of unity for the Ge minimum yield [Fig. 1(a)], for both normal (squares) and off-normal ($\langle 11\bar{1}\rangle$ direction, triangles) incidence. For comparison the solid and dash-dotted lines describe the expected decrease in Ge minimum yield for incidence along $\langle 111\rangle$ and $\langle 11\bar{1}\rangle$, respectively, under the assumption of perfect epitaxy. (Up to $\approx 4$ ML pseudomorphic growth would be expected[6] on the basis of van der Merwe's theory of epitaxy for a nonreconstructed surface.) The calculations, carried out by means of numerical simulations, assumed a one-dimensional root mean square vibrational amplitude of 0.0870 Å without surface enhancement and correlation coefficients of 0.475 and 0.0 for next-nearest neighbors along $\langle 111\rangle$ strings separated by short and long distances, respectively.[7]

Although the Ge layer appears disordered as measured by LEED and ion scattering, we cannot rule out the existence of short-range order in which the Ge overlayer is configured in small domains, each domain consisting of a crystallite with a reconstructed surface. Since the surface reconstruction of Ge(111) is known to extend $\approx 4$ ML into the bulk, such a configuration, in the coverage range investigated, would give a value of the minimum yield not significantly different from a truly amorphous layer. However, in either case, no significant shadowing of the Si substrate by the Ge overlayer is expected and indeed none is observed, as can be seen from the constant SP value in Fig. 1(b) and 1(c). This observation agrees basically with the normal-incidence data of Narusawa and Gibson[8] and Narusawa, Gibson, and Hiraki[9]; however, we do not observe the slight increase in the Si SP intensity for Ge coverages of $\approx 2$ ML, as was reported by them.[9]

It is remarkable that the Si(111)-$(7\times7)$ surface structure seems essentially unperturbed by the deposition of a few-monolayer-thick Ge overlayer. Qualitatively, this behavior is inconsistent with a simple relaxation model of this surface.[3] Vertical displacements can be expected to be strongly affected by the presence of a few-monolayer-thick film. On the other hand, stacking-fault geometries and features of a rough reconstruction[10,11] might be preserved for room-temperature deposition.

For the Si(100)-$(2\times1)$ surface, too, the Ge minimum yield does not show any order in the overlayer [Fig. 1(d)], either in normal (squares) or in off-normal $\langle\bar{1}\bar{1}1\rangle$ (triangles) incidence. For comparison the solid and dash-dotted lines show simulation results for perfect epitaxy. (A correlation coefficient of 0.15 was assumed for $\langle 100\rangle$ strings.) Again, this strong evidence for a disordered overlayer is supported by the LEED pattern which vanishes beyond $\approx 2.2$ ML, as indicated in the bottom part of Fig. 1(f).

In striking contrast to the Si(111)-$(7\times7)$ case, however, the Si(100) SP intensity [Figs. 1(e), 1(f)] does not remain at the clean-surface value but drops in a practically linear fashion until it reaches the respective bulk values for normal and off-normal incidence [the horizontal part of the solid line in Figs. 1(e) and 1(f)], whereupon no further change occurs with increasing coverage. This is perfectly consistent with deposition of a disordered Ge overlayer on top of a reconstructed Si(100)-$(2\times1)$ surface and the simultaneous reordering of the Si surface to a bulklike structure.

In principle, the reduction of the Si SP intensity measured in normal incidence [Fig. 1(e)] might be attributed to shadowing by an epitaxial overlayer. However, an analogous reduction of the Si SP intensity is found for off-normal incidence [Fig. 1(f)] where, even for a perfect epitaxial Ge film, shadowing is unlikely because of the tetragonal distortion expected for such an overlayer.[6] Furthermore, we already found compelling evidence, which was described above, that the Ge film is highly disordered, which excludes any shadowing in the first place. The behavior of the Si SP intensity with Ge coverage [Fig. 1(e) and 1(f)], therefore, is typical for the reordering of the substrate.

A simple phenomenological model can be used to describe this reordering by a disordered layer [solid line in Figs. 1(b), 1(c), 1(e), and 1(f)]. It assumes that $\Theta$ monolayers of Ge relieve $\Theta$ monolayers of Si reconstruction until at a Ge-coverage $\Theta_c$ the substrate is completely reordered and its SP intensity has reached its bulk value $I^{SP}_{bulk}$. In the absence of shadowing the SP intensity will then stay constant beyond $\Theta_c$ at $I^{sp}_{bulk}$. $\Theta_c$ is given from the SP intensity of the clean surface, $I^{SP}_{clean}$, as $\Theta_c = k(I^{SP}_{clean} - I^{SP}_{bulk})$ where $k$ denotes the number of monolayers visible to the incident beam in a particular channeling direction. For $\Theta < \Theta_c$ the model SP intensity versus coverage curve is therefore a straight line through the points $(0, I^{SP}_{clean})$ and $(\Theta_c, I^{SP}_{bulk})$.

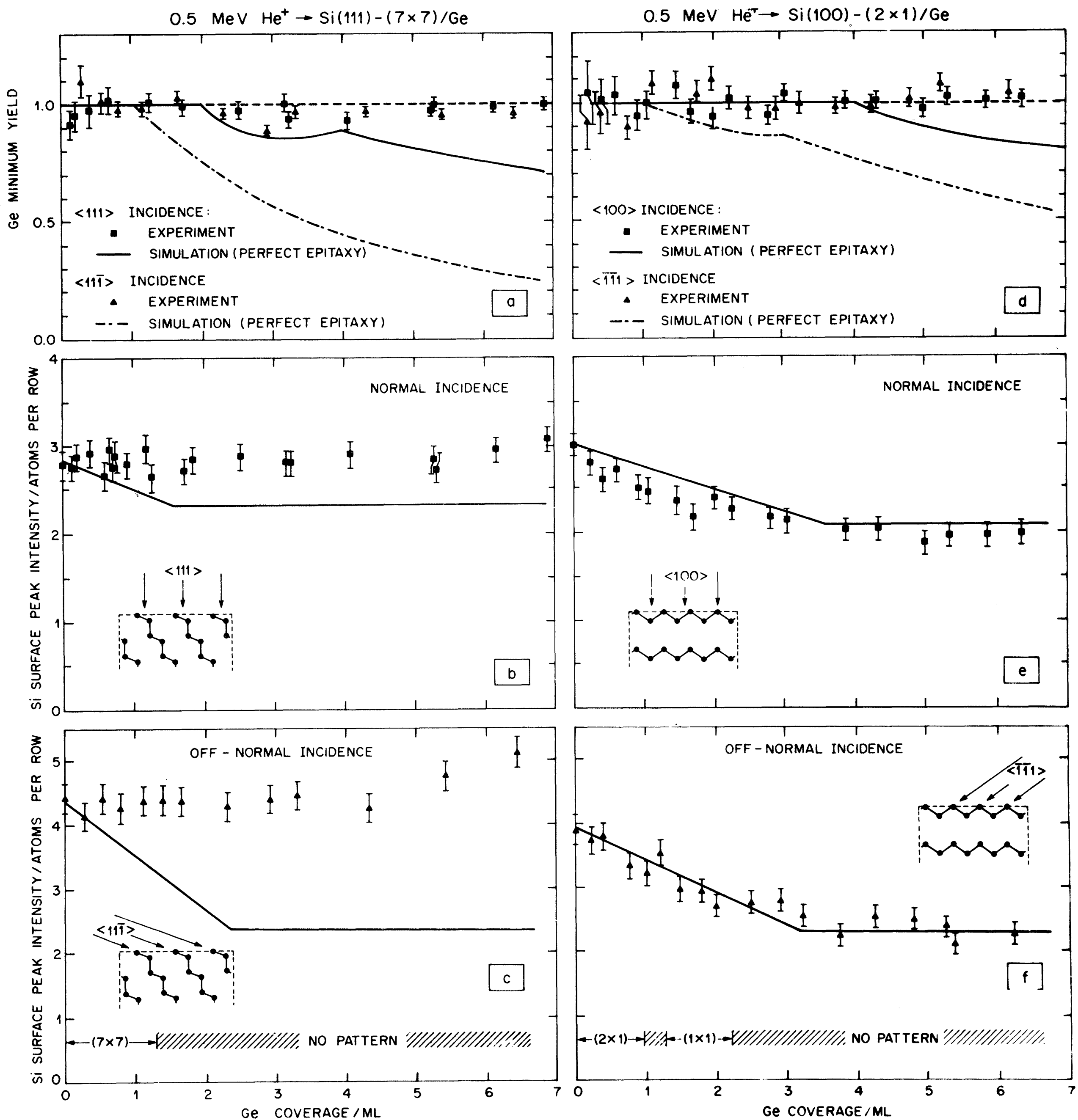


FIG. 1. Comparison of Ge minimum yield (first row) and Si surface peak intensities in normal (second row) and off-normal (third row) incidence between (a)–(c) the Ge covered Si(111)-(7×7) and (d)–(f) the Si(100)-(2×1) surface. In (b), (c), (e), and (f) the solid lines show the expected behavior of the surface peak intensity if the Ge overlayer reorders the substrate, removing the displacements linearly with coverage, and no shadowing by the overlayer occurs. Insets schematically show the alignment of the incident $He^+$ beam with respect to the sample (side view). The bottom part of (c) and (f) qualitatively indicates the observed LEED pattern.

The agreement with the model (solid line) is very good for normal incidence [Fig. 1(e)], where $k=4$, and even better for off-normal incidence [Fig. 1(f)], where the sensitivity for displacements is higher ($k=2$) and any accidental shadowing, not detectable from the Ge minimum-yield measurements, is less likely to occur because of the tetragonal distortion expected for the Ge film.[6] Note that no free parameters enter the

model. In contrast, the experimental results for Si(111)-(7×7) in Figs. 1(b) and 1(c) do not show any decrease at all towards a more bulklike substrate; this is especially apparent for $\langle 11\bar{1}\rangle$ incidence [Fig. 1(c)], where $k = 1$.

We conclude that room-temperature Ge deposition reorders the Si(100)-(2×1) surface in a linear way, but is unable to transform the Si(111)-(7×7). At present the preferred structure model for the Si(100)-(2×1) is the formation of asymmetric[12] surface dimers[13] with sizable subsurface strain[14] (i.e., a weak reconstruction), while for the Si(111)-(7×7) recent work[10,11,15] favors a strong reconstruction. For the Si(100)-(2×1) surface a breaking of the dimer bonds without any mass transfer would be required to reach a bulklike configuration, while the strong reconstruction of the (7×7) would necessarily involve the actual movement of Si atoms across the surface. It is then not implausible that the room-temperature deposition of Ge is able to reorder the Si(100)-(2×1) but not the Si(111)-(7×7), and one would expect that raising the substrate temperature during deposition should overcome this barrier. We note[16] that, indeed, deposition at temperatures beyond $\approx 300\,°C$ causes the reordering of the Si(111)-(7×7), the Si SP intensity following closely the solid lines in Figs. 1(b) and 1(c), in complete analogy to Si(100)-(2×1).

In conclusion, our measurements demonstrate that the room-temperature deposition of Ge on the Si(100)-(2×1) and Si(111)-(7×7) reconstructed surfaces causes Si reordering in the former but not in the latter case; we ascribe this difference to the different nature of the reconstruction.

We acknowledge discussions with J. C. Bean, Y. J. Chabal, A. T. Fiory, Y. Kuk, E. G. McRae, S. Nakahara, and I. K. Robinson and the technical support of P. J. Silverman.

[1]L. C. Feldman, CRC Crit. Rev. Solid State Mater. Sci. Mater. **10**, 143 (1981).

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

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

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

[5]H.-J. Gossmann, J. C. Bean, L. C. Feldman, and W. M. Gibson, Surf. Sci. **138**, L175 (1984).

[6]J. C. Bean, L. C. Feldman, A. T. Fiory, S. Nakahara, and I. K. Robinson, J. Vac. Sci. Technol. A **2**, 436 (1984).

[7]O. H. Nielsen, University of Aarhus Internal Report, 1979 (unpublished).

[8]T. Narusawa and W. M. Gibson, Phys. Rev. Lett. **47**, 1459 (1981).

[9]T. Narusawa, W. M. Gibson, and A. Hiraki, Phys. Rev. B **24**, 4835 (1981).

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

[11]G. Binning, H. Rohrer, Ch. Gerber, and E. Weibel, Phys. Rev. Lett. **50**, 120 (1983).

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

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

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

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

[16]H.-J. Gossmann, L. C. Feldman, and W. M. Gibson, to be published.