Observation of a (2×8) surface reconstruction on $Si_{1-x}Ge_x$ alloys grown on (100) Si by molecular-beam epitaxy

E. T. Croke
California Institute of Technology, Pasadena, California 91125

R. J. Hauenstein[a)]
Hughes Research Laboratories, Malibu, California 90265

T. C. Fu and T. C. McGill
California Institute of Technology, Pasadena, California 91125

(Received 2 February 1991; accepted 11 April 1991)

We present evidence supporting the formation of a new, (2×8) surface reconstruction on $Si_{1-x}Ge_x$ alloys grown on (100) Si substrates by molecular-beam epitaxy. Surfaces of $Si_{1-x}Ge_x$ alloys were studied using reflection high-energy electron diffraction (RHEED) and low-energy electron diffraction (LEED) techniques. RHEED patterns from samples with Ge concentrations, x, falling within the range 0.10–0.30 and grown at temperatures between 350 and 550 °C, exhibit $n/8$ fractional-order diffraction streaks in addition to the normal (2×1) pattern seen on (100) Si. The presence of fractional-order diffracted beams is indicative of an eight-fold-periodic modulation in electron scattering factor across the alloy surface. LEED patterns from surfaces of samples grown under similar conditions are entirely consistent with these results. In addition, the LEED patterns support the conclusion that the modulation is occurring in the direction of the dimer chains of a (2×1) reconstruction. We have examined the thermal stability of the (2×8) reconstruction and have found that it reverts to (2×1) after annealing to 700 °C and reappears after the sample temperature is allowed to cool below 600 °C. Such behavior suggests that the reconstruction is a stable, ordered phase for which the pair-correlation function of surface Ge atoms exhibits an eightfold periodicity in the "1" direction of a Si-like (2×1) reconstruction. We also present a simulation in the kinematic approximation, confirming the validity of our interpretation of these findings.

I. INTRODUCTION

Interest in the $Si_{1-x}Ge_x$/Si material system has increased dramatically in recent years primarily because of the enormous potential for fabricating novel, heterojunction devices compatible with existing Si-based processing technologies. Recent results[1,2] point to material quality as the single, most important factor in determining device performance; therefore, a study of the physical mechanisms of epitaxial growth is extremely timely. Once these mechanisms are understood, growth conditions can be adjusted to produce the highest-quality material possible. Toward this aim, our studies have focused on surfaces of $Si_{1-x}Ge_x$ alloys grown epitaxially on (100) Si substrates by molecular-beam epitaxy (MBE).

In this paper, reflection high-energy electron diffraction (RHEED) and low-energy electron diffraction (LEED) techniques are used to study the surface reconstruction of $Si_{1-x}Ge_x$ alloys grown on (100) Si substrates. Most of the samples studied were grown below the 550 °C empirical, critical thickness curve of People and Bean[3] with the exception of one that was deliberately relaxed through the use of a high-temperature anneal. RHEED and LEED patterns from these surfaces indicate the presence of a (2×8) surface reconstruction with the "8" direction aligned perpendicular to the dimerization direction. (2×n) reconstructions have been observed previously on clean (100) Si after a quenching from high temperatures[4,5] and on (100) Si contaminated with Ni (Ref. 6) and Cu (Ref. 7) impurities. Our samples have been determined through the use of secondary-ion mass spectroscopy (SIMS) and x-ray photoelectron spectroscopy (XPS) to be free from any metallic impurities.

We present experimental evidence suggesting that the (2×8) reconstruction is a thermodynamically favored arrangement of surface dimers ordering in a direction perpendicular to the dimerization direction of a (2×1) Si surface reconstruction. Similar models have previously been proposed to explain the (100) Si (2×n) reconstructions. Martin *et al.*[5] concluded that these reconstructions result from ordered phases of missing-dimer defects, a conclusion based on an earlier treatment by Pandey.[8] Further refinements to this model made by Aruga and Murata[9] detail a mechanism for ordering arising from lattice strain surrounding the defects. In our model, Ge dimers play the same role as the missing-dimer defects. Local strains surrounding each Ge dimer drive the reconstruction toward the ordered phase. Presumably, an optimal configuration exists when Ge dimers are located at every eighth site. In order to support our conclusions, we present simulated diffraction patterns from one-dimensional atomic chains. The calculated patterns are consistent with the interpretation that the fractional-order peaks observed experimentally are due to ordered Ge dimers on the surface. Finally, simulations including strain effects are shown to qualitatively predict the relative intensities of the fractional order peaks.

 0734-211X/91/042301-06$01.00

II. EXPERIMENT

A. Surface preparation by MBE

Experimental observations of surface reconstructions were performed through the use of three independent MBE growth systems. LEED images were produced in a custom-built ultrahigh-vacuum (UHV) chamber with a base pressure $<8\times10^{-11}$ Torr and typical growth pressures of approximately 5×10^{-9} Torr. Si and Ge were coevaporated onto heated, 2-in. Si substrates. A more complete description of this growth system is described elsewhere.[10] RHEED patterns from similarly prepared samples were observed in a Perkin-Elmer 430S Si MBE system (base pressure $<1\times10^{-10}$ Torr). Here, Si and Ge were codeposited from a dual *e*-beam source onto heated, 3-in. Si substrates. Si and Ge fluxes were simultaneously monitored by a cathodoluminescent flux sensor (Inficon, Sentinel III). An identical Perkin-Elmer system was used to corroborate the results obtained in these two growth chambers.

The samples used in this study were prepared using standard MBE growth techniques. First, (100) Si substrates were degreased in (1,1,1)-trichloroethane, acetone, and methanol solvents at a temperature of approximately 50 °C. The substrates were subsequently rinsed in de-ionized water and etched in 50% HF in order to remove any SiO_2 present on the surface. After the etch, the substrates were again rinsed in de-ionized water and removed slowly, eliminating the need to dry the samples with nitrogen since the etched Si is hydrophobic. Recently, we have used this technique since we have felt that blow-drying the substrates needlessly introduces particulates on the surface. After degreasing, the substrates were immediatedly loaded into the MBE growth chamber. Once inside the vacuum system, the substrates were heated to approximately 850 °C and exposed to a nominally 0.1 Å/s Si flux for approximately 2 min in order to assist in the removal of any remaining oxide.[11,12] Following oxide desorption, a buffer layer of Si, several hundred Angstroms thick, was grown as the substrate temperature was ramped down from 700 to 500 °C. In this way, atomically clean Si starting surfaces were prepared rather routinely.

B. *In situ* surface analysis techniques

The surface periodicities of our samples were analyzed *in situ* through the use of RHEED and LEED analytical techniques. As indicated above, LEED patterns were obtained from samples grown in a custom-built MBE growth chamber. The apparatus consists of a Princeton Research Instruments reverse-view LEED optical system mounted on a 6-in. flange adjacent to the sample heater. Typical beam energies ranged from 30 to 100 eV. Patterns appearing on the phosphor screen were photographed with a Nikon (Model F3/T) 35-mm camera loaded with 3200 ASA film. RHEED patterns were obtained from samples grown in the Perkin-Elmer Si MBE growth chambers. In this case, a 10-keV electron beam was diffracted from the sample at glancing incidence. Patterns were recorded digitally through the use of a Cohu solid-state charge-coupled device (CCD) camera, an S-VHS video recorder, an Analogic (Model DASM) frame grabber, and a Sun SPARC™ station. Each image consists of a 512×512 array of single-byte data (0.26 MB/frame). Recording the images in this way allows a great deal of flexibility in analyzing the data. For instance, several rows of data can be selected and averaged together in order to improve signal to noise and accurately measure the separation between streaks in a RHEED pattern.

III. RESULTS

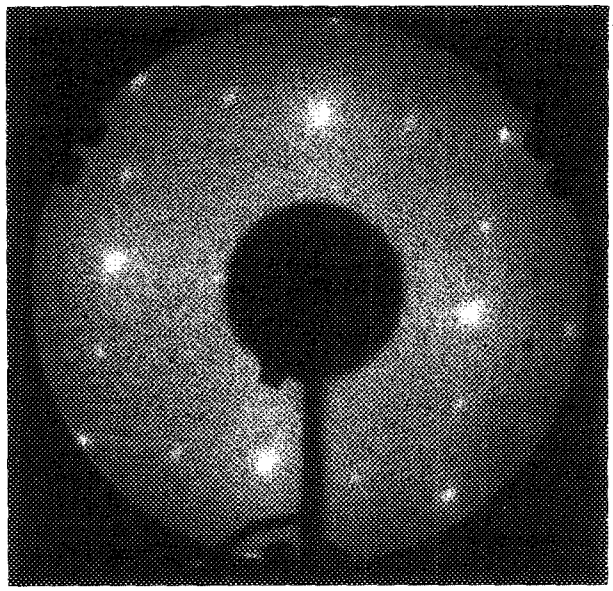
A. LEED observations

As discussed earlier, samples for this study were grown on (100) Si substrates that were degreased and etched in a 50% HF solution prior to loading into the UHV deposition chamber. Once inside the growth chamber, an atomically clean Si surface was prepared through the use of an *in situ* oxide-desorption procedure followed by growth of a pure Si buffer layer. The LEED pattern from a sample prepared in this way is shown in Fig. 1(a). Integer and half-integer order spots are clearly visible in the figure. Such a pattern is typically observed on pure Si-reconstructed surfaces that contain roughly equal mixtures of (2×1) and (1×2) domains.[13] Although it is possible to obtain a single-domain (2×1) reconstruction on a Si surface,[13,14] such an attempt was not undertaken here. Consequently, Fig. 1(a) represents an incoherent superposition of the diffraction patterns from (2×1) and (1×2) domains. Henceforth, references to $(m\times n)$ surface symmetries should be understood to refer to incoherent superpositions of $(m\times n)$ and $(n\times m)$ symmetries.

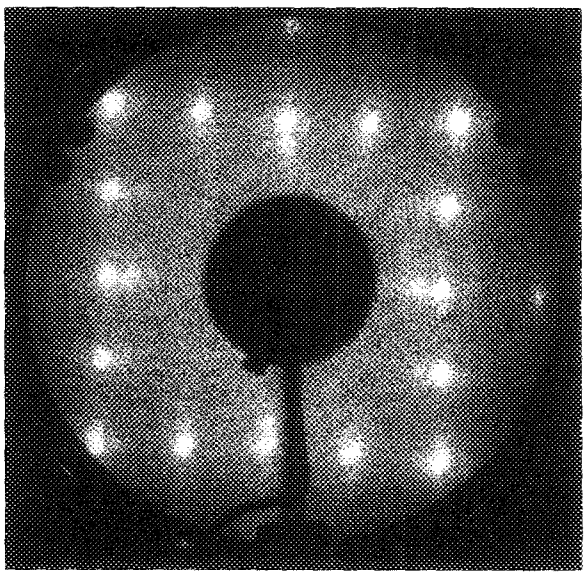
After we obtained a clean (2×1) Si surface, 200-Å $Si_{0.82}Ge_{0.18}$ were deposited onto the substrate at a temperature of approximately 550 °C. The LEED pattern from this sample is shown in Fig. 1(b). Visible in the figure are additional fractional-order diffraction spots located near integer and half-integer spots of the (2×1) reconstruction. The presence of fractional-order spots suggests that a long-range periodicity is present on the surface. The fact that only one set of fractional-order spots occur near each half-integer spot indicates that the long-range periodicity is aligned with the direction of the dimer chains of a pure Si (2×1) reconstruction.[15] Finally, as the energy of the electron beam was varied, all spots in the pattern moved and did not break up, eliminating the possibility that steps could be responsible for the observed reconstruction.[16]

B. RHEED observations

Surface reconstructions observed with RHEED from samples grown in the two Perkin-Elmer MBE systems are entirely consistent with our LEED observations. In order to investigate the compositional dependence of the ordered reconstruction, several $Si_{1-x}Ge_x$ samples were grown at the fixed temperature of 450 °C and at a deposition rate of approximately 1 Å/s. Samples for which the Ge composition x lies within the range 0.10–0.30 consistently exhibit the usual (2×1) Si reconstruction modified by the appearance of fractional-order beams. For samples in which x lies outside this range, the reconstruction is (2×1). The RHEED pattern from a $Si_{0.80}Ge_{0.20}$ surface grown under these conditions was recorded digitally and studied in order to deter-



(a)



(b)

FIG. 1. (a) LEED pattern from a clean (100) Si surface. Integer and half-integer diffraction spots are visible due to the usual (2×1) reconstruction. (b) Diffraction pattern from a 200-Å $Si_{0.82}Ge_{0.18}$ alloy grown by MBE at approximately 550 °C on a clean (100) Si substrate. Fractional-order spots suggest the presence of a periodic modulation in electron scattering factor occurring in a direction parallel to the dimer chains normally seen on clean (100) Si surfaces. Electron beam energy for both patterns is approximately 47 eV.

mine the exact position of the fractional-order streaks. Fifteen lines of data were averaged together and plotted in Fig. 2. The improved signal-to-noise ratio resulting from the averaging process reveals all fractional orders as shoulders against a strong background. The indicated peak positions were identified through the use of a numerical peak-finding algorithm.[17] Since there are seven equally spaced fractional-order peaks between each integer order, we conclude that the reconstruction is eightfold periodic. Taking into consideration our LEED results, we conclude that the observed reconstruction periodicity is (2×8).

The surface of another sample intentionally grown at low

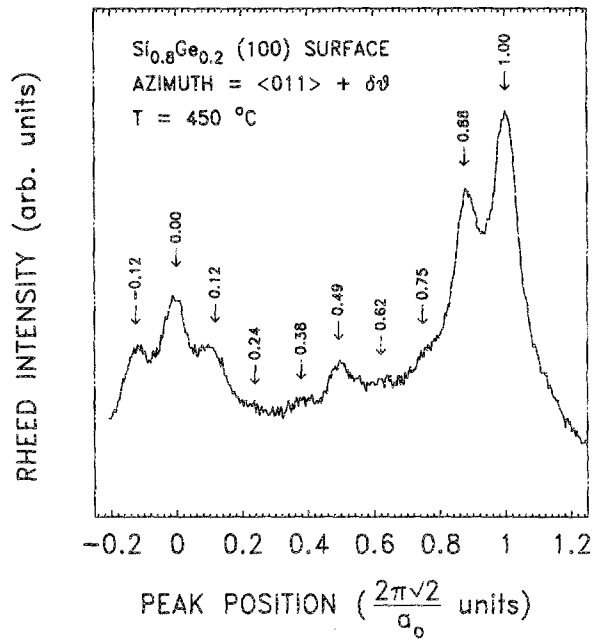


FIG. 2. Plot of RHEED Intensity vs peak position for a 200-Å $Si_{0.80}Ge_{0.20}$ grown at 450 °C. Fifteen lines of data were averaged together in order to improve signal to noise so that an accurate measurement of the peak spacings could be made. Peak positions were identified with the aid of a numerical peak-finding algorithm, verifying the eightfold-periodic nature of the reconstruction.

temperature was studied to determine the thermal stability of the (2×8) reconstruction. The RHEED pattern from a 200-Å $Si_{0.80}Ge_{0.20}$ sample grown at 230 °C is shown in Fig. 3(a). As indicated by the spots in the pattern, the sample surface immediately after growth was very rough. The sample was subsequently heated to 700 °C in 10 min. As the temperature climbed above 450 °C, the RHEED pattern improved considerably. The spots were replaced by sharp streaks, indicating that the surface had become smooth. Also, fractional-order streaks became visible. At 700 °C, the fractional-order peaks became difficult to see, perhaps due to thermal diffuse scattering. After the anneal, the heater power was cut off and the sample temperature was allowed to "freefall" back to room temperature. The RHEED pattern taken after the anneal is shown in Fig. 3(b). The fractional-order streaks were sharper after the anneal than they were while the temperature was rising to the anneal temperature. Since a high-temperature anneal did not destroy the ordering in the reconstruction, we can conclude that it is thermodynamically stable.

One of our samples was deliberately grown in excess of the critical thickness in order to check the dependence of bulk strain on the appearance of the (2×8) reconstruction. A 5000-Å $Si_{0.80}Ge_{0.20}$ layer grown at 450 °C displayed a sharp (2×8) reconstruction immediately after growth. A 3-h anneal at 700 °C was used to relax the sample. Previous studies[18,19] have shown that such a film should relax approximately 84% of coherent strain under these conditions. After the anneal, the (2×8) pattern was still present, suggesting that bulk strain does not appear to affect the formation of this reconstruction. Conclusive evidence of the effect of strain on the formation of the (2×8) reconstruction re-

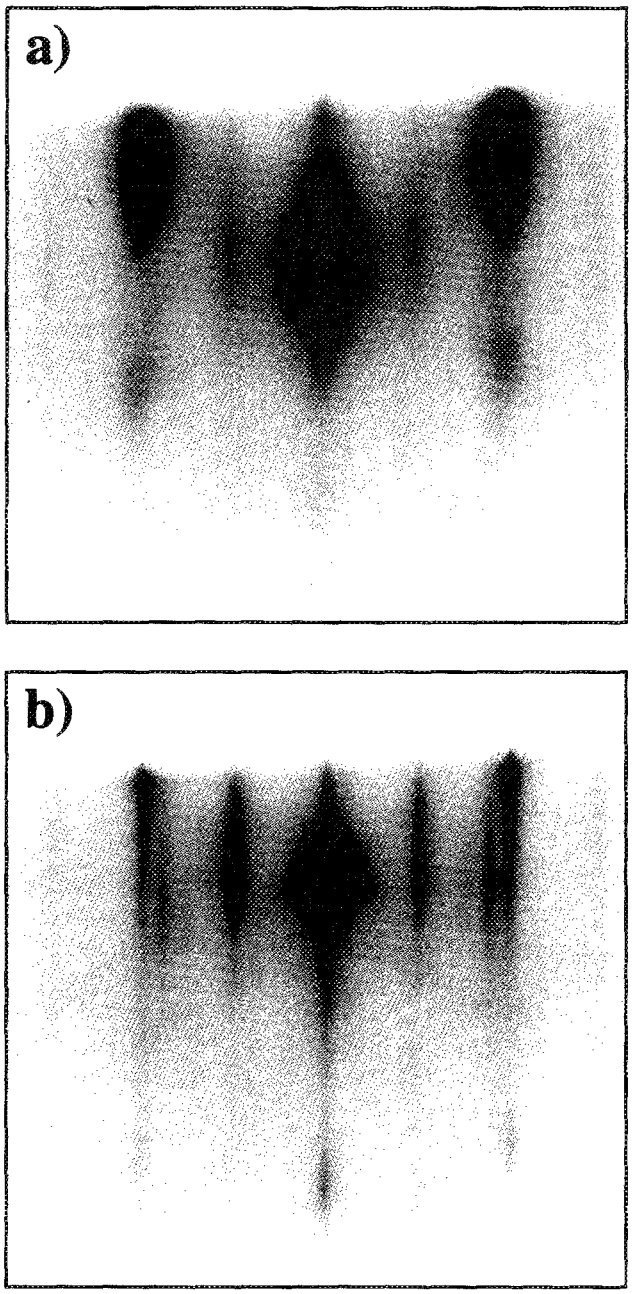


FIG. 3. (a) RHEED pattern from a 200-Å $Si_{0.80}Ge_{0.20}$ alloy grown at 230 °C. Growth at low temperature has resulted in a rough surface, producing a spotty pattern. (b) RHEED pattern from the same sample after a brief anneal to 700 °C. The sharp streaks in the pattern indicate that the sample surface has become smooth. Atoms have rearranged on the surface, reproducing the same ordering phenomena observed with LEED.

mains elusive, since the annealed sample is still approximately 16% strained. It should be pointed out that the pattern after the anneal was not as sharp as before the anneal, possibly because of disorder created by the introduction of large numbers of threading dislocations during the relaxation process.

We have also observed the evolution of the RHEED pattern on a (100) Si substrate under a slight Ge flux. First, a sharp (2×1) pattern was obtained through the use of the usual desorption procedure and subsequent Si buffer layer growth. Then, at a temperature of 500 °C, the surface was exposed to a 0.01-Å/s Ge flux. After about 160 s (1 monolayer), the reconstruction changed from (2×1) to (2×8). The ordered reconstruction persisted until a total of approximately 5 monolayers of Ge were deposited. At this point, the reconstruction became faceted, possibly due to the formation of Ge islands. Interestingly enough, a further deposition of Si reversed the process exactly. The faceted pattern reverted to (2×8) and then, after nearly 10 monolayers of Si, became (2×1). It is interesting to note that several monolayers were necessary to cause the reconstructions to change, suggesting that some segregation had taken place during growth. The behavior described above demonstrates that Ge plays a very important role in the formation of the (2×8) reconstruction. Indeed, the reconstruction can be created and destroyed simply by changing the surface Ge concentration.

IV. KINEMATICAL CALCULATION OF DIFFRACTION FROM AN ORDERED LINEAR CHAIN

We propose the following model for the (2×8) $Si_{1-x}Ge_x$ surface reconstruction based on the ordered defect model proposed by Martin *et al.*[5] to explain the origin of (2×*n*) reconstructions observed on (100) Si. In our model, ordering of Ge dimers in a direction perpendicular to the dimerization direction locates them approximately eight atoms apart. Arranging these ordered dimer chains by lining up the Ge dimers in the "2" direction yields the required (2×8) symmetry. Composition can be adjusted as necessary without affecting the symmetry by randomly substituting one type of atom for the other. In order to evaluate the validity of this model, we have approximated the ordered dimer chain as an ordered linear chain of individual scattering sites. Finally, we have simulated electron diffraction from such a chain through the use of the kinematic approximation.[20]

Each atom in the chain is defined by a position, $\mathbf{r}_n$, and a form factor, f_n, describing the relative strength of interaction with the incident electron beam. Si atoms are arbitrarily assigned a form factor of 1. Ge atoms, however, receive a value of 2.3 since the form factor is known to vary approximately linearly with atomic number.[20,21] Also, since the diffracting electrons are coherent over a distance of several hundred angstroms,[21] we have limited the number of atoms involved in the calculation to 160. The intensities of the diffracted beams are a function of the difference in wavevector between the scattered electrons and the incident electrons. Hence, we define $\mathbf{k}$ such that

$$\mathbf{k} = \mathbf{k}_{\text{out}} - \mathbf{k}_{\text{in}}. \tag{1}$$

In our model, each scatterer contributes a phase multiplied by its form factor to the overall scattering intensity, $I(\mathbf{k})$, which can be written

$$I(\mathbf{k}) = \left| \sum_n f_n e^{i\mathbf{k}\cdot\mathbf{r}_n} \right|^2. \tag{2}$$

Using Eq. (2), we have calculated $I(\mathbf{k})$ for an ordered linear chain in order to study the effect of strain on the relative intensities of the fractional order peaks.

In the unstrained case, each scatterer is located exactly 1 unit apart. The calculated diffraction pattern appears in Fig.

4(a). Intensity has been normalized so that at k = 0, it takes on a value of 1. It should be pointed out that each fractional order peak is exactly the same intensity. The strained case is shown in Fig. 4(b). Here, the Si—Si bond length has been decreased while the Si—Ge bond length has been increased. The eight-atom unit cell length, of course, was preserved. In the figure, notice that the intensity of the $\frac{7}{8}$-order peak has increased relative to the $\frac{9}{8}$-order peak. This is consistent with our experimental results. In the unphysical case where the Si—Ge bond length is made to be *shorter* than the Si—Si bond length, the intensity of the $\frac{7}{8}$-order peak decreases relative to the $\frac{9}{8}$-order peak. These results support our contention that Ge dimers are ordering along the direction of the dimer chains of a (2×1) reconstruction.

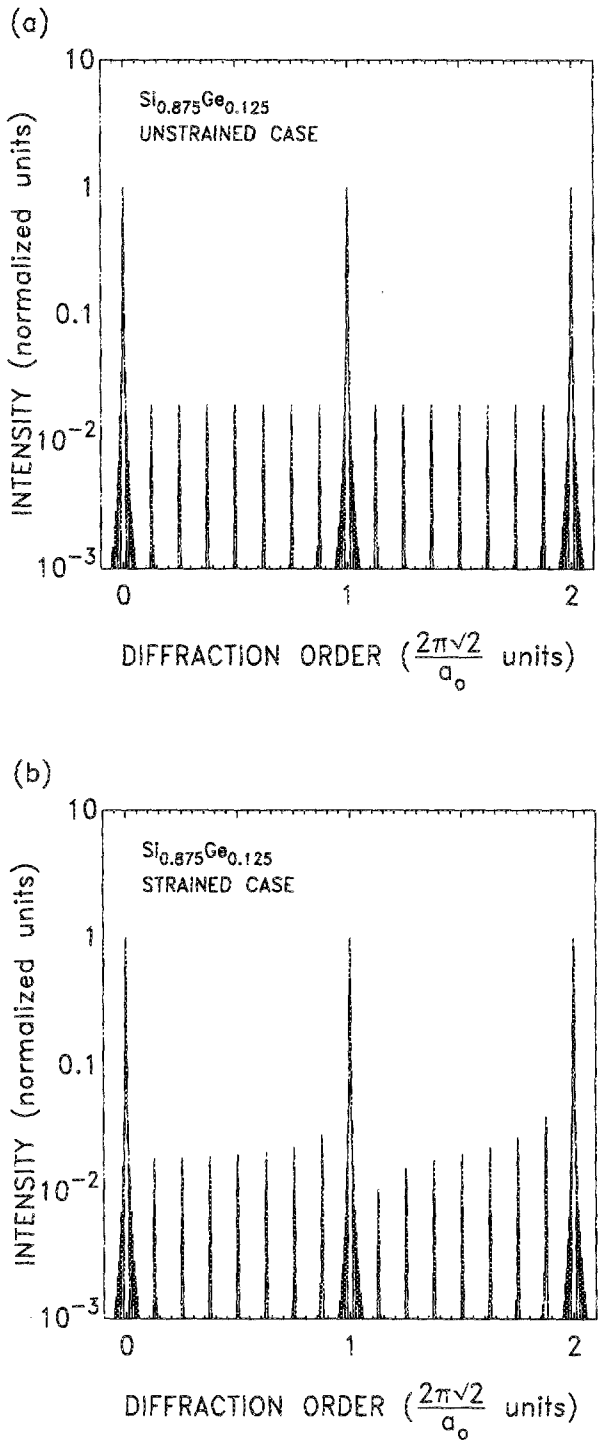


FIG. 4. (a) Simulated diffraction pattern from an ordered chain of Si and Ge atomic scatterers in which Ge atoms are located every eight atomic positions. Visible in the figure are fractional-order diffraction peaks of equal intensity. (b) Diffraction from a similar chain of atoms in which Si—Ge bond lengths were chosen to be slightly larger than Si—Si bond lengths. The increase in $\frac{7}{8}$-order peak intensity relative to $\frac{9}{8}$-order intensity is consistent with RHEED and LEED observations.

V. DISCUSSION

Our observations indicate that within the compositional range $0.10 \leqslant x \leqslant 0.30$, RHEED and LEED patterns from $Si_{1-x}Ge_x$ alloys grown at temperatures between 350 and 550 °C exhibit a (2×8) surface reconstruction. Under these growth conditions, the patterns show no evidence of faceting or islanding. In the case of faceting, additional streaks at an angle to the original Si-surface streaks would appear in the RHEED pattern and are not observed. Islanding, on the other hand, would produce a spotty RHEED pattern because of the increasingly three-dimensional nature of the surface. Our surfaces exhibit sharply streaked RHEED patterns, and hence no evidence of island growth is observed.

Recently, several authors have suggested that Ge should segregate in the first few monolayers of a $Si_{1-x}Ge_x$ alloy surface, resulting in a surface Ge concentration considerably in excess of the bulk concentration.[22,23] We have not attempted to measure the concentration of the surface Ge atoms in our samples. Nevertheless, in view of the previously reported results, it still is our contention that Ge is ordering on the alloy surface. In the case of a Ge-rich surface, our results can be explained in terms of ordering of missing-dimer defects, similar to the model proposed by Aruga and Murata[9] for the Si (2×*n*) reconstructions. The kinematical calculation presented earlier yields roughly identical results for the Ge-rich chain missing Ge atoms every eight atomic positions. In fact, the calculation still predicts the correct relative intensities of the fractional-order peaks if strain effects are included.

Quantitative prediction of the intensity of the fractional-order diffraction streaks is not possible in the kinematic approximation. A more precise calculation would necessarily involve the effects of multiple scattering, inelastic scattering, and temperature, and hence is beyond the intended scope of this paper. In addition, the real surface may deviate significantly from perfect (2×8) order. In this case, the calculated diffraction pattern would predict an enhancement of the $(n \pm \frac{1}{8})$-order peak intensities over the other fractional-order peak intensities. Since we have observed the sharpness of the (2×8) reconstruction to vary with growth and annealing conditions, significant deviation from perfect (2×8) symmetry is likely to exist, accounting for any differences in the observed and calculated diffraction patterns.

VI. CONCLUSIONS

We have observed a (2×8) surface reconstruction on surfaces of $Si_{1-x}Ge_x$ alloys grown on (100) Si for compositions

x between approximately 0.10 and 0.30. Outside this compositional range, RHEED and LEED patterns exhibit a (2×1) Si-like reconstruction. We have also investigated the thermal stability of the reconstruction and found it to persist even after a high-temperature anneal, suggesting that it is thermodynamically stable. Our results demonstrate that simply changing the surface concentration of Ge influences the type of reconstruction present. These results lead us to conclude that Ge is ordering on the surface. We suspect that the Ge atoms are arranging themselves in dimers that order in a direction perpendicular to the dimerization direction. A repulsive force due to local lattice strains between Ge dimers may be responsible for the observed ordering phenomenon. This conclusion is similar to the model proposed by Aruga and Murata[9] to explain the mechanism of missing-dimer defect ordering on (100) Si. Finally, results from our simulation are consistent with this model since the intensity of the $\frac{7}{8}$-order peak increases relative to that of the $\frac{2}{8}$-order peak for atomic chains including strain effects.

ACKNOWLEDGMENTS

One of us, E. T. Croke, would like to acknowledge International Business Machines Corporation for support under a graduate research fellowship. In addition, the authors would like to acknowledge the partial support of the Office of Naval Research under Grant No. N00014-89-J-3196.

[a] Present address: Physics Dept., Oklahoma State University, Stillwater, OK 74078.

[1] E. F. Crabbé, G. L. Patton, J. M. C. Stork, J. H. Comfort, B. S. Meyerson, and J. Y.-C. Sun, IEDM Tech. Dig., 17 (1990).
[2] D. L. Harame, J. M. C. Stork, B. S. Meyerson, E. F. Crabbé, G. J. Scilla, E. de Frésart, A. E. Megdanis, C. L. Stanis, G. L. Patton, J. H. Comfort, A. A. Bright, J. B. Johnson, and S. S. Furkay, IEDM Tech. Dig., 33 (1990).
[3] R. People and J. C. Bean, Appl. Phys. Lett. **47**, 322 (1985); **49**, 229 (1986).
[4] K. Muller, E. Lang, L. Hammer, W. Grim, P. Heilman, and K. Heinz, in *Determination of Surface Structure by LEED*, edited by P. M. Markus and F. Jona (Plenum, New York, 1984), p. 483.
[5] J. A. Martin, D. E. Savage, W. Moritz, and M. G. Lagally, Phys. Rev. Lett. **56**, 1936 (1986).
[6] K. Kato, T. Ide, S. Miura, A. Tamura, and T. Ichinokawa, Surf. Sci. **194**, L87 (1988).
[7] L. Barbier and J. Lapujoulade, J. Vac. Sci. Technol. A **8**, 2662 (1990).
[8] K. C. Pandey, in *Proceedings of the Seventeenth International Conference on the Physics of Semiconductors*, edited by D. J. Chadi and W. A. Harrison (Springer, New York, 1985), p. 55.
[9] T. Aruga and Y. Murata, Phys. Rev. B **34**, 5654 (1986).
[10] R. J. Hauenstein, Ph.D. thesis, California Institute of Technology, 1987.
[11] C. F. Huang, R. P. G. Karunasiri, K. L. Wang, and T. W. Kang, in *Proceedings of the Second International Symposium on Silicon Molecular Beam Epitaxy*, edited by J. C. Bean and L. J. Schowalter (The Electrochemical Society, Pennington, 1988), p. 501.
[12] D. Striet and F. Allen, J. Appl. Phys. **61**, 2894 (1987).
[13] C. E. Aumann, D. E. Savage, R. Kariotis, and M. G. Lagally, J. Vac. Sci. Technol. A **6**, 767 (1988).
[14] T. Sakamoto and G. Hashiguchi, Jpn. J. Appl. Phys. **25**, L78 (1986).
[15] E. T. Croke, R. J. Hauenstein, T. C. Fu, and T. C. McGill (unpublished).
[16] M. A. van Hove, W. H. Weinberg, and C.-M. Chan, *Low Energy Electron Diffraction: Experiment, Theory, and Surface Determination* (Springer, Berlin, 1986).
[17] A. Savitsky and M. J. E. Golay, Anal. Chem. **36**, 1627 (1964).
[18] R. J. Hauenstein, B. M. Clemens, R. H. Miles, O. J. Marsh, E. T. Croke, and T. C. McGill, J. Vac. Sci. Technol. B **7**, 767 (1989).
[19] R. J. Hauenstein, R. H. Miles, E. T. Croke, and T. C. McGill, Thin Solid Films **183**, 79 (1989).
[20] P. B. Hirsch, A. Howie, R. Nicholson, D. W. Pashley, and M. J. Whelan, *Electron Microscopy of Thin Crystals* (Krieger, Malabar, FL, 1977), pp. 85–107.
[21] J. B. Pendry, *Low Energy Electron Diffraction* (Academic, London, 1974).
[22] P. C. Kelires and J. Tersoff, Phys. Rev. Lett. **63**, 1164 (1989).
[23] J. E. Rowe, D. M. Riffe, and G. K. Wertheim, presented at the Eighteenth Conference on the Physics and Chemistry of Semiconductor Interfaces, Long Beach, CA, January 29–February 1, 1991.