Surface electronic structure of Si(111)7×7-Ge and Si(111)5×5-Ge studied with photoemission and inverse photoemission

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Angle-resolved photoemission and inverse photoemission have been used to study the electronic structure of Si(111)7×7-Ge and Si(111)5×5-Ge surfaces. For both surfaces, one unoccupied and three occupied surface-state bands have been mapped along the $\bar{\Gamma}$-$\bar{K}$ and $\bar{\Gamma}$-$\bar{M}$ lines in the 1×1 surface Brillouin zone. These bands have characteristics similar to those of the surface-state bands observed for the clean Si(111)7×7 surface. Quantitative differences in the dispersions seem to correlate with the Ge content in the surfaces rather than with surface periodicity.

I. INTRODUCTION

During the last few years there has been a growing interest in the properties of semiconductor-semiconductor interfaces, Ge on Si(111) being one of the prototypical systems. High-energy ion scattering and electron diffraction studies[1-3] have shown that Ge films deposited on Si(111)7×7 surfaces at room temperature (RT) are amorphous, and that there is no intermixing or island formation. For temperatures above ~500 °C, epitaxial Ge films can be grown, but at these temperatures there is significant intermixing of Ge and Si.[1,2] When approximately two monolayers (ML)[4] of Ge are deposited onto a Si(111)7×7 surface at 400–700 °C, a surface with a 5×5 reconstruction is obtained.[2,5] Also surfaces of Ge_xSi_{1-x} alloys[2] and surfaces obtained by annealing RT deposits of ~2 ML of Ge on a clean Si(111) surface[5-7] exhibit a 5×5 reconstruction. Low-energy electron diffraction[8] (LEED) and scanning tunneling microscopy[9] (STM) studies of the Si(111)5×5-Ge surface indicate strong similarities with the clean Si(111)7×7 surface. Very recently, a transmission electron-diffraction experiment on the 5×5-Ge surface[10] has confirmed that this surface has an atomic structure similar to the dimer adatom stacking-fault (DAS) structure of the clean 7×7 surface.[11]

Recent electron energy-loss spectroscopy (EELS) and LEED studies of annealed Ge deposits on clean Si(111)7×7 surfaces have shown that there exists a Si(111)7×7-Ge surface with a different 7×7 LEED pattern and different EELS spectra than for the clean 7×7 surface.[7,12] The Si(111)7×7-Ge surface was obtained either by annealing a Si(111)5×5-Ge surface at ~870 °C or by deposition of ~1.5 ML of Ge at temperatures above 400 °C.

In a recent paper[13] we presented results of an angle-resolved ultraviolet photoelectron spectroscopy (AR-UPS) study of Si(111)7×7-Ge and Si(111)5×5-Ge surfaces. For the 7×7-Ge surface, three surface states were identified with characteristics similar to the corresponding surface states on the clean Si(111)7×7 surface. For the 5×5-Ge surface, only two surface states could be clearly identified, but there was some evidence of a third state. In this paper, we report on a more extensive AR-UPS study using synchrotron radiation. The existence of the third surface state on the 5×5-Ge surface is confirmed, and the initial-energy dispersions of the three occupied surface states on the two Ge-covered surfaces are determined along the high-symmetry lines in the surface Brillouin zone. In addition, **k**-resolved inverse photoelectron spectroscopy (KRIPES) is used to map the dispersion of an unoccupied band on both surfaces. The results are compared with those obtained for the clean Si(111)7×7 surface.

II. EXPERIMENTAL DETAILS

The angle-resolved photoemission experiment was performed on a VG Scientific ADES 400 spectrometer using polarized synchrotron radiation from the DORIS II storage ring (Doppel-Ring Speicheranlage) at Hamburger Synchrotronstrahlungslabor, Deutsches Elektronen-Synchrotron.[14] All spectra presented in this paper have been recorded with the polarization vector of the light parallel to the plane in which the electrons were analyzed. The estimated total energy resolution as determined by the analyzer voltages and the monochromator slit widths was ~0.15 eV and the angular resolution of the analyzer was ±2°. The position of the Fermi level was determined to an accuracy of ±0.05 eV by photoemission from the metallic sample holder. The base pressure in the vacuum system was better than 2×10^{-10} Torr.

The inverse-photoemission spectra were recorded using a Geiger-Müller type photon detector with a SrF_2 window (9.5 eV pass energy). The total energy resolution (electrons and photons) was ~0.35 eV and the divergence of the electron beam was smaller than ±1.5° (corresponding to a momentum resolution better than 0.1 $Å^{-1}$).[15] The position of the Fermi level was deter-

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mined to an accuracy of ±0.05 eV by inverse photoemission from a polycrystalline Ta foil. The base pressure in the vacuum system was better than 5×10^{-11} Torr.

Figure 1 shows the geometry of the 1×1 surface Brillouin zone (SBZ) of the Si(111) surface. All photoemission and inverse-photoemission spectra presented in this paper were recorded along a $[10\bar{1}]$ azimuthal direction, which corresponds to a $\bar{\Gamma}$–$\bar{K}$ line in the 1×1 SBZ, but spectra have also been recorded along $[11\bar{2}]$ and $[2\,\bar{1}\,\bar{1}]$ directions, corresponding to $\bar{\Gamma}$–$\bar{M}$ lines.

The samples used in the present experiments were cut from lightly *n*-doped mirror-polished Si wafers ($\rho\sim5$ Ω cm, $N_D\sim1\times10^{15}$ cm^{-3}). The surface normal was off by less than 0.2° from the [111] direction. Before insertion into the vacuum chamber, the samples were degreased and etched according to the procedure by Henderson.[16] In ultrahigh vacuum the samples were thoroughly outgassed at ~500 °C, heated to ~950 °C for 10 min, and then annealed at ~700 °C for 5 min. This procedure gives clean surfaces showing sharp 7×7 LEED patterns. Ge of 99.999% purity was evaporated from thoroughly outgassed tungsten filaments at a rate equivalent to ~1 ML/min, as monitored with a quartz microbalance. During Ge evaporation and annealing of the samples, the pressure in the vacuum chamber was better than 3×10^{-10} Torr.

Prior to the photoemission and inverse-photoemission experiments, we studied the preparation of Si(111)7×7-Ge and Si(111)5×5-Ge surfaces by annealing of thin Ge deposits on clean Si(111)7×7 surfaces. This was done in a separate ultrahigh-vacuum chamber equipped with an electron-beam-heated source for Ge evaporation and facilities for Auger-electron spectroscopy (AES), reflection high-energy electron diffraction (RHEED), and LEED.

III. RESULTS AND DISCUSSION

A. Auger-electron spectroscopy

When Ge is deposited onto a clean Si(111)7×7 surface at room temperature, the intensity of the 92-eV Si(*LVV*) Auger transition shows an exponential decay,[2,6,17] indicating that the Ge overlayer grows uniformly, without island formation or indiffusion. By fitting the experimentally determined Si(*LVV*) Auger peak intensities as a function of Ge coverage to an exponential curve, we have found a value of λ~2.5 ML for the mean free path of 92-eV electrons in the Ge overlayer. This value is in good agreement with the value found by Gossmann *et al.*[2] (~2.4 ML), while Chen *et al.*[17] obtained a slightly larger value (~3.1 ML).

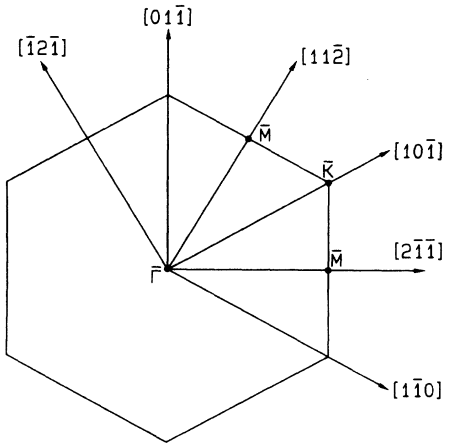

FIG. 1. Geometry of the 1×1 surface Brillouin zone of the Si(111) surface.

Figure 2(a) shows the intensities of the 92-eV Si(*LVV*) and 52-eV Ge(*MMM*) Auger peaks as functions of annealing temperature for a room-temperature deposition of ~4.2 ML of Ge onto a clean Si(111)7×7 surface. The intensities have been normalized to the intensities obtained for pure reference materials. The annealing time is 1 min at each temperature. In Fig. 2(b) the normalized intensities of the Si(*LVV*) and Ge(*MMM*) peaks are shown as functions of annealing time for a fixed temperature of 850 °C and an initial Ge coverage of ~4.6 ML. Also shown in Figs. 2(a) and 2(b) are the observed changes in the LEED pattern. The gradual growth of the Si peak and decrease of the Ge peak can be due either to the formation of Ge islands on top of the surface or to intermixing of Si and Ge. Another possible explanation is that Ge is evaporated, but this effect should be small at least for the lowest temperatures.

From the curves in Figs. 2(a) and 2(b) it is possible to estimate the Ge content in the outer layers of surfaces showing a 5×5 or a 7×7 LEED pattern, either assuming a pure Ge overlayer (giving an upper limit of the Ge content at the surface) or assuming a homogenous alloy within the probe depth. For the assumption of a pure Ge overlayer, the coverage is obtained from the normalized Si(*LVV*) AES signal and the experimentally determined inelastic mean free path λ (~2.5 ML). This gives a Ge coverage of 1.3–3.0 ML for surfaces showing a 5×5 LEED pattern, and a coverage of up to 1.1 ML for surfaces showing a 7×7 pattern. These results are consistent with previous studies of Ge overlayers of Si(111)7×7 using AES[6,7] and core-level photoelectron spectroscopy.[18]

Assuming a homogenous alloy within the AES probe depth, the Ge content can be calculated as the normalized Ge(*MMM*) Auger intensity divided by the sum of the normalized Ge(*MMM*) and Si(*LVV*) intensities (in this way no account is taken for possible matrix effects on the relative sensitivities of the Si and Ge Auger peaks). This results in a Ge concentration of 30–70% for surfaces showing a 5×5 reconstruction, and up to ~24% for surfaces showing a 7×7 reconstruction. These results can be compared with results obtained by Gossmann *et al.*[3] for (111) surfaces of Ge_xSi_{1-x} alloys. For alloys with compositions ranging from $x=28\%$ to $x=69\%$ a 5×5 reconstruction was observed, in agreement with the present work. For an alloy containing 14% of Ge a mixed 5×5 and 7×7 LEED pattern was observed.[3] This is a much lower Ge content than the ~28% found for mixed surfaces in the present study. It is quite possible that this discrepancy is due only to the difference in method of surface preparation. However, it

is also possible that the Ge content in the overlayers is somewhat overestimated in the present study due to the neglect of matrix effects. Another factor that might be of importance is surface segregation of Ge in the Ge_xSi_{1-x} alloys, which could cause a higher Ge concentration at the surface of the alloy than in the bulk.

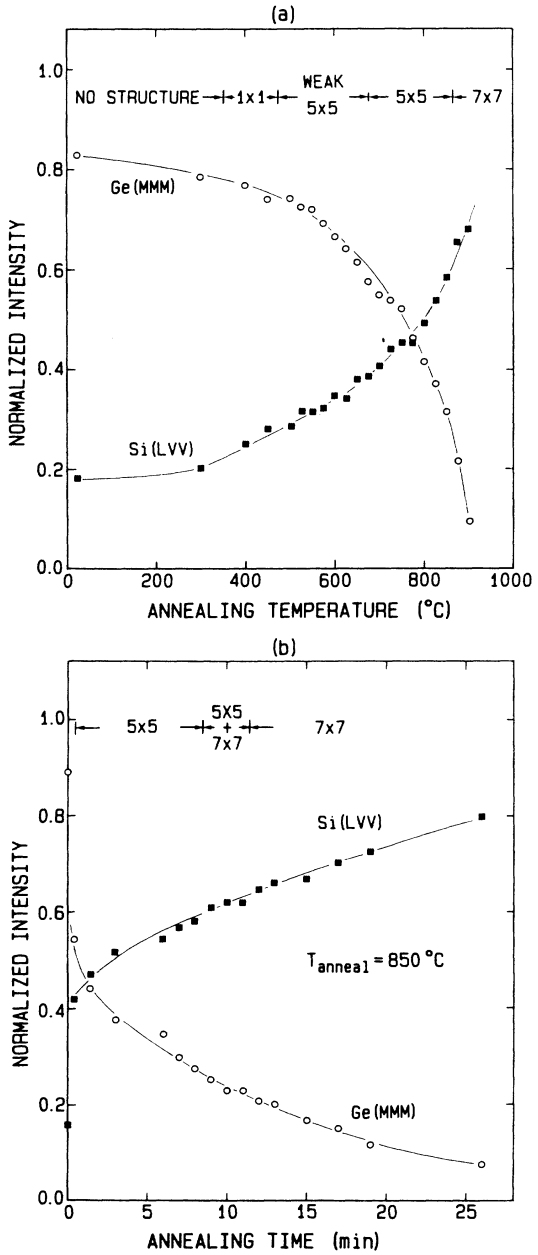

FIG. 2. (a) Dependence of the normalized intensity of the 92-eV Si(*LVV*) (■) and 52-eV Ge(*MMM*) (○) Auger-electron spectroscopy (AES) signals on annealing temperature for a room-temperature deposition of ~4.2 ML of Ge. The annealing time was 1 min for each temperature. (b) Dependence of the normalized intensity of the 92-eV Si(*LVV*) (■) and 52-eV Ge(*MMM*) (○) AES signals on annealing time for a room-temperature deposition of ~4.5 ML of Ge. The annealing temperature was 850 °C.

In Figs. 2(a) and 2(b) there are no flat regions, which would have indicated that there is an optimal Ge content at which the 5×5-Ge and/or 7×7-Ge surfaces occur. Such a flat region was, however, reported for the 5×5-Ge surface in the study by Shoji *et al.*[6] This was interpreted as evidence that the 5×5 structure is due to 2 ML of pure Ge on top of the Si(111) surface.[6] A possible reason for the reported differences in annealing behavior is the use of different annealing times. In the study in Ref. 6 the samples were annealed 10 min at each temperature.

From the Auger-intensity measurements, it is difficult to draw any conclusions regarding the lateral uniformity of the annealed Ge-covered surfaces. However, we have found no evidence for island formation in the electron-diffraction studies, i.e., the RHEED patterns have not shown the bulk diffraction that would result from three-dimensional islands, and LEED shows a mixed pattern only over a very limited Ge-concentration range. Thus there is no indication that the surfaces would be inhomogenous. Further, the present study shows that there are significant quantitative differences between the electronic properties of the Ge-covered surfaces and those of the clean Si(111)7×7 surface, indicating that substantial amounts of Ge must be distributed uniformly over the 5×5-Ge and 7×7-Ge surfaces.

B. Photoemission and inverse photoemission

ARUPS spectra recorded from the clean Si(111)7×7 surface at 21.2-eV photon energy are shown in Fig. 3 for various angles of emission along the [10$\bar{1}$] azimuthal direction. As previously reported,[19–21] the structures S_1, S_2, and S_3 are due to emission from surface states. The S_1 state, at ~0.20 eV below the Fermi level (E_F), has a maximum in emission intensity for $\theta_e = 15°$. The S_2 state is positioned at ~0.95 eV below E_F in normal emission, but has a small (~0.15 eV) upwards dispersion with maximum energy at $\theta_e = 15°$. The surface state S_3 is not clearly visible for angles of emission $\theta_e < 15°$, but for angles of emission $\theta_e > 17.5°$ it shows a downwards dispersion with an observed bandwidth of ~0.30 eV.

Figure 4 shows ARUPS spectra recorded at 21.2-eV photon energy from the Si(111)5×5-Ge surface. This surface was prepared by evaporating ~4 ML of Ge onto a clean Si(111)7×7 surface, followed by approximately 5 min annealing at ~700 °C, resulting in a sharp 5×5 LEED pattern with low background. In the spectra we have identified three surface-state structures, B_1, B_2, and B_3, although in Fig. 4 it appears as if there is just one state in the energy range 1.0–1.5 eV below E_F. The state B_2, observed at ~1.05 eV below E_F, is clearly visible close to normal emission, while the B_3 state is pronounced for large emission angles. For angles between 10° and 15°, the emission from the B_2 state overlaps with emission from B_3 and it is not possible to separate the observed peak into different contributions in the spectra shown. However, in other spectra, recorded with different photon energies, different polarizations, and along different azimuthal directions (not shown), it is clear that there are two separate surface states in this en-

ergy range. The states B_1 and B_2 show no significant initial-energy dispersion, while the B_3 state has a downwards dispersion with an observed bandwidth of ~ 0.30 eV.

In a recent angle-integrated photoemission study of the Si(111)5×5-Ge surface, Miller *et al.*[22] observed a surface state positioned at the Fermi level. This state corresponds to the B_1 state in the spectra shown in Fig. 4. In the angle-integrated spectrum in Ref. 22, the main peak is rather broad and no clear feature corresponding to either the B_2 or the B_3 state can be identified.

In Fig. 5, ARUPS spectra recorded from the Si(111)7×7-Ge surface are shown. The surface was prepared by annealing the Si(111)5×5-Ge surface at ~ 800 °C, while the surface was repeatedly checked with LEED. After several minutes the first 7×7 spots started to appear, and after a total time of approximately 10 min a sharp 7×7 LEED pattern with low background had developed and all traces of the 5×5 reconstruction were gone. This method of preparation was chosen in order to obtain a 7×7-Ge surface with the largest possible Ge content. In the spectra it is possible to identify three surface-state structures, A_1, A_2, and A_3. The two nondispersing states A_1 and A_2 are observed at ~ 0.20 and ~ 1.05 eV below E_F, respectively. The A_3 state has a downwards dispersion with an observed bandwidth of ~ 0.35 eV.

The spectra recorded from the Si(111)7×7-Ge and Si(111)5×5-Ge surfaces are rather similar. The main difference is that the surface state A_3 for the 7×7-Ge surface is positioned ~ 0.2 eV lower in initial energy than the corresponding B_3 state for the 5×5-Ge surface. Because of this, the A_2 state is visible (as a shoulder) for large angles of emission. The surface state S_3 for the clean Si(111)7×7 surface is positioned ~ 0.25 eV lower in energy than the A_3 state, and the S_3 and S_2 states are not overlapping. The S_2 state is therefore clearly observable for almost all emission angles.

Although there are significant differences in initial-energy positions of the lowest-lying surface states on the three surfaces, the widths of the S_3, A_3, and B_3 peaks in the photoemission spectra are very similar. Moreover, ARUPS spectra have been recorded for several 5×5-Ge and 7×7-Ge surfaces, obtained starting from surfaces with somewhat different *initial* amounts of Ge, and the results show that the electronic structures of these surfaces are reproducible. These observations are indicative of the lateral uniformity of the Ge-covered surfaces,

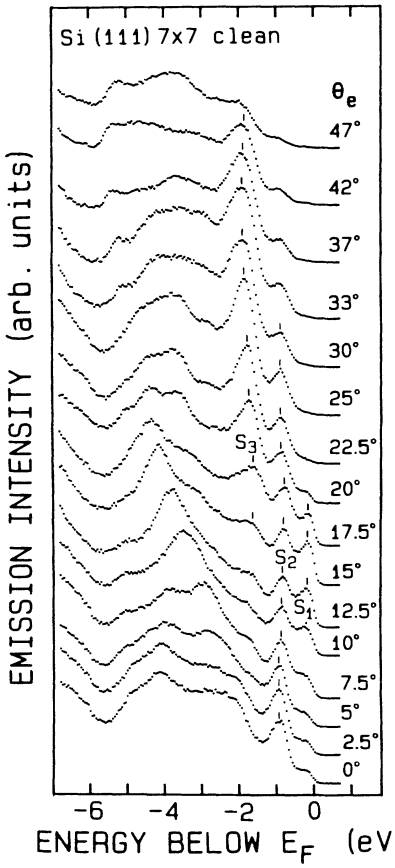

FIG. 3. Photoemission spectra recorded from Si(111)7×7 with 21.2 eV photon energy for various angles of emission along the [10$\bar{1}$] azimuthal direction. The angle of incidence is $\theta_i = 45°$.

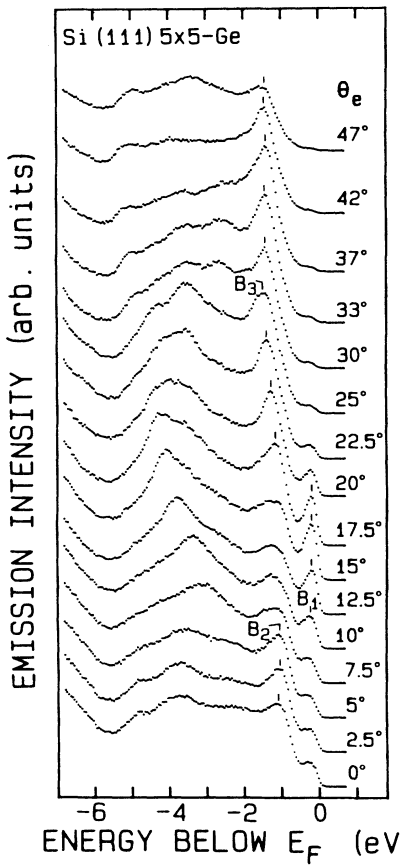

FIG. 4. Photoemission spectra recorded from Si(111)5×5-Ge with 21.2 eV photon energy for various angles of emission along the [10$\bar{1}$] azimuthal direction. The angle of incidence is $\theta_i = 45°$.

since a nonuniformity should result in less well-defined dispersions of the surface states, causing an increased width of the surface-state peaks.

For binding energies higher than ~ 2.0 eV, the spectra recorded from the clean Si(111)7×7 surface are dominated by structures due to emission from bulk states.[21] These structures are also present for the Ge-covered surfaces, with approximately the same initial energies as for the clean surface. This indicates that the change in band bending due to the evaporated Ge is small (<0.15 eV).

ARUPS spectra from the three surfaces have also been recorded along $[11\bar{2}]$ and $[2\bar{1}\bar{1}]$ azimuthal directions, corresponding to $\bar{\Gamma}$–$\bar{M}$ lines in the SBZ (see Fig. 1). In these spectra (not shown) the same surface-state structures are observed as in the spectra in Figs. 3–5, recorded along a $\bar{\Gamma}$–$\bar{K}$ line. The behavior of the surface states S_{1-3}, A_{1-3}, and B_{1-3} along the $\bar{\Gamma}$–$\bar{M}$ lines is very similar to the behavior along $\bar{\Gamma}$–$\bar{K}$, except for two things. First, the minima of the initial-energy dispersions of the lowest-lying surface states S_3, A_3, and B_3 are located ~ 0.15 eV lower in energy along the $\bar{\Gamma}$–$\bar{M}$ directions as compared to the $\bar{\Gamma}$–$\bar{K}$ direction. The second difference is that, along $\bar{\Gamma}$–$\bar{M}$, the states close to the Fermi level (S_1, A_1, and B_1) are observable not only for angles of emission around 15°, but also for large angles of emission (around 45°).

The surface-state structures S_1, S_2, and S_3 are suppressed if the angle of incidence of the light is reduced, indicating that the states have p_z character.[21] ARUPS spectra recorded from Si(111)7×7-Ge and Si(111)5×5-Ge surfaces using unpolarized 10.2-eV radiation at normal incidence show that states A_1, A_2, A_3, B_1, and B_3 have p_z character as well.[13] For 10.2-eV photon energy the surface state B_2 could not be observed and the character of this state has not been determined.

Inverse-photoemission spectra recorded along the $[10\bar{1}]$ azimuthal direction from Si(111)7×7-Ge and Si(111)5×5-Ge surfaces are shown in Figs. 6 and 7, respectively. The surfaces were prepared in the same manner as described above for the surfaces used in the ARUPS experiment. The structures A for the 7×7-Ge surface and B for the 5×5-Ge surface are due to transi-

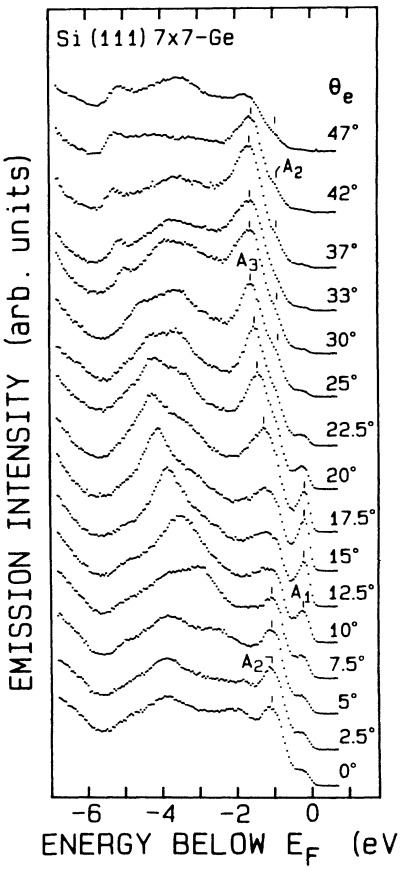

FIG. 5. Photoemission spectra recorded from Si(111)7×7-Ge with 21.2 eV photon energy for various angles of emission along the $[10\bar{1}]$ azimuthal direction. The angle of incidence is $\theta_i = 45°$.

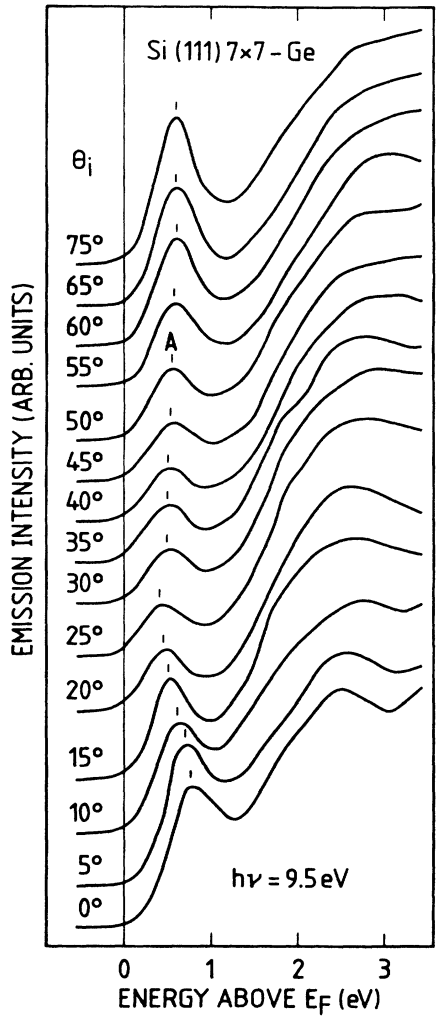

FIG. 6. Inverse-photoemission spectra recorded from the Si(111)7×7-Ge surface for various angles of incidence along the $[10\bar{1}]$ azimuthal direction.

tions into empty surface states which are located well within the projected bulk band gap. The energy dispersions of these empty states are very similar. For normal incidence, the energy positions of states A and B are ~ 0.80 eV and ~ 0.70 eV above E_F, respectively. For increasing angles, the states disperse towards the Fermi level, and reach a minimum energy, ~ 0.40 eV above E_F, for $\theta_i = 25°$. For even larger angles the states disperse upwards again, by ~ 0.20 eV. The emission patterns of structures A and B are also very similar, with high intensities for incidence angles corresponding to $k_\parallel$ values around the center and boundary of the 1×1 surface Brillouin zone, and low intensities for incidence angles around $\theta_i = 25°$. For $\theta_i = 30°$ the experimental geometry is such that mainly photons emitted in the normal direction are detected, while the angle between the emitted photons and the normal direction increases for higher and lower incidence angles. Therefore the observed emission patterns could be due to a p_z character of states A and B.

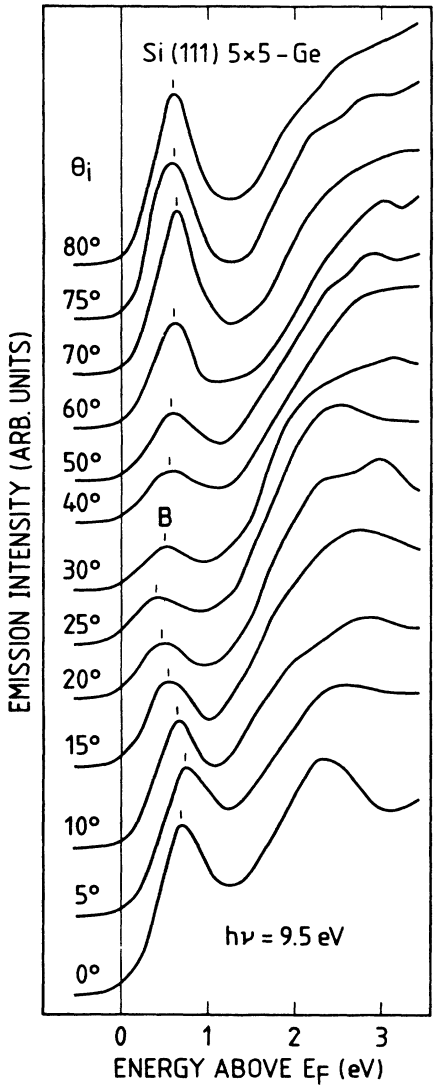

FIG. 7. Inverse-photoemission spectra recorded from the Si(111)5×5-Ge surface for various angles of incidence along the $[10\bar{1}]$ azimuthal direction.

In the KRIPES spectra recorded along the $[11\bar{2}]$ and $[2\,\bar{1}\,\bar{1}]$ azimuthal directions (not shown) the surface-state structures A and B can be observed with quite similar dispersions and emission patterns as described above for the $[10\bar{1}]$ direction. The behavior of states A and B is qualitatively similar to the behavior found for a pronounced empty surface state S at the clean Si(111)7×7 surface.[23] An important difference between states A and B and state S is, however, that the total dispersion of state S is significantly smaller (~ 0.20 as compared to ~ 0.40 eV).

Figures 8(a) and 8(b) show the experimental energy dispersions of the filled and empty surface states of the Si(111)7×7-Ge and Si(111)5×5-Ge surfaces, respectively. Also shown in the figures are the experimental dispersions of the surface states of the clean Si(111)7×7 surface.[24] The dispersion of the empty state S for the clean surface is from Ref. 23.

From the dispersions in Figs. 8(a) and 8(b) it is clear that the electronic properties of the Si(111)7×7, Si(111)7×7-Ge, and Si(111)5×5-Ge are qualitatively very similar. The similarity between the clean 7×7 and the 5×5-Ge surfaces is consistent with the similarity observed in experiments probing the geometric structure of these surfaces.[8–10] The gradual change in electronic structure going from the clean 7×7 surface via the 7×7-Ge to the 5×5-Ge surface seems to correlate with the Ge content on the surfaces rather than with the surface periodicity. Especially, the dispersions of the empty state A and the second filled state A_2 on the 7×7-Ge surface are more similar to the dispersions of the corresponding states B and B_2 on the 5×5-Ge surface than to the dispersions of states S and S_2 on the clean 7×7 surface.

Although the peak positions of states S_1, A_1, and B_1 are ~ 0.2 eV below the Fermi level, it is clear that there is finite emission intensity at the Fermi level in the AR-UPS spectra for the clean as well as the Ge-covered surfaces. This is also true for spectra recorded at higher energy resolution using 10.2-eV radiation.[13] In those spectra the S_1, A_1, and B_1 surface states can be clearly observed for all $k_\parallel$ values along the high-symmetry lines in the 1×1 SBZ, although the maxima in emission intensity occur at the same points in the SBZ as for the 21.2-eV spectra. Also in the inverse-photoemission spectra (Figs. 6 and 7), there is intensity at the Fermi level, though rather weak. Evidence for a metallic character of the clean Si(111)7×7 surface (apart from the finite emission intensity at E_F in photoemission and inverse-photoemission spectra[19–21,23,25]) has been obtained with electron energy-loss spectroscopy.[26–28] From the present photoemission and inverse-photoemission studies, it seems clear that the Si(111)7×7-Ge and Si(111)5×5-Ge surfaces have metallic character as well, in agreement with the result for the 5×5-Ge surface in the angle-integrated photoemission study by Miller *et al.*[22] At the Fermi level, the density of states is higher than indicated by the spectra, since the Fermi-

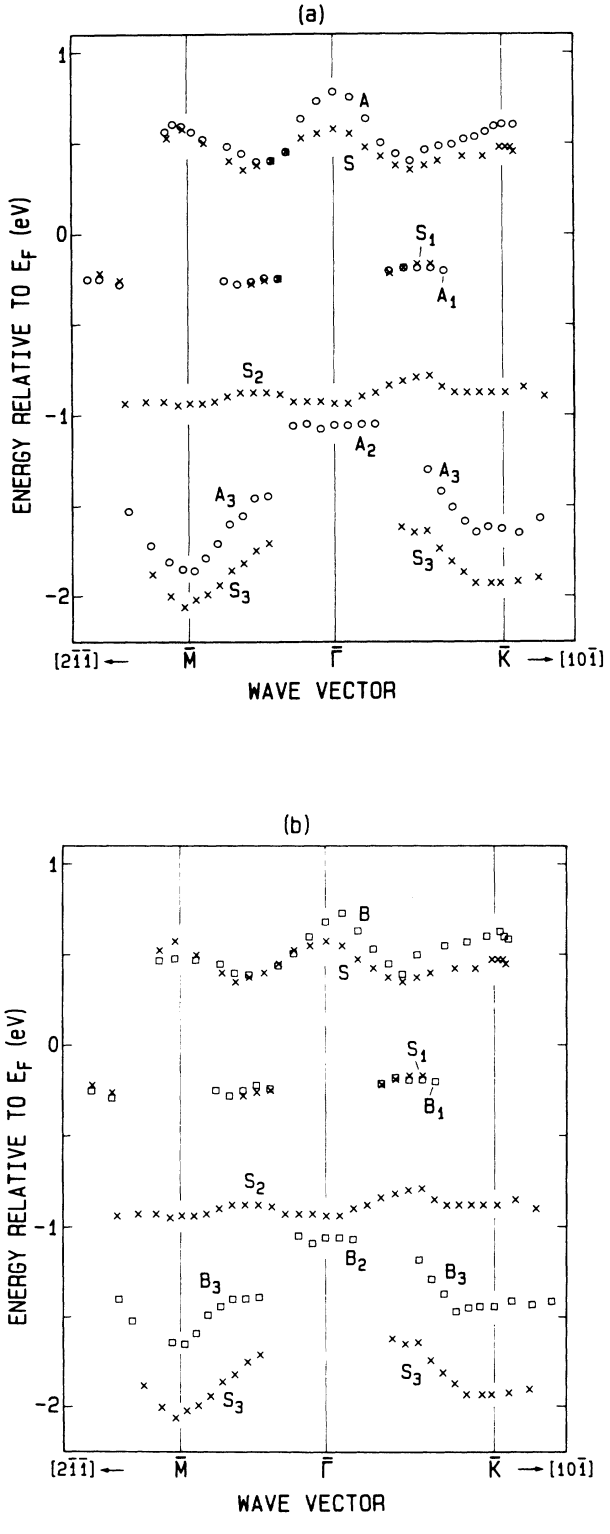

FIG. 8. (a) Experimental energy dispersions of the filled and empty surface states for the Si(111)7×7-Ge surface (○) and the clean Si(111)7×7 surface (×) along the $[10\bar{1}]$ and $[2\bar{1}\bar{1}]$ azimuthal directions. (b) Same as (a) but for the Si(111)5×5-Ge surface (□) and the clean Si(111)7×7 surface (×). The dispersion of the empty state S for the Si(111)7×7 surface is from Ref. 23.

level distribution will lower the emission intensity. Even if this effect is taken into account, the density of surface states at the Fermi level appears to be rather low for the clean and Ge-covered surfaces. For all three surfaces, a quite large energy separation (0.5–0.6 eV) is found between the dispersions of the highest occupied band (S_1, A_1, and B_1) and the unoccupied band (S, A, and B).

Currently, the most generally accepted model for the clean Si(111)7×7 surface is the so-called dimer adatom stacking-fault (DAS) model, derived by Takayanagi *et al.*[11] from results of transmission electron-diffraction experiments. The results of recent x-ray diffraction[29] and scanning tunneling microscopy[30] experiments on Si(111)7×7 seem to be consistent with the DAS model. In a recent spectroscopic STM study, Hamers *et al.*[31] have resolved the various surface states of the Si(111)7×7 surface in real space and interpreted the results in terms of the DAS model. A partly filled state observed close to the Fermi level was assigned to the dangling bonds on the 12 adatoms in the surface unit cell. This state corresponds to the state S_1 seen in photoemission and the metallic tail seen in inverse photoemission. A state observed around 0.5 eV above E_F, corresponding to the empty state S, was also assigned to the adatoms, while the filled state corresponding to S_2 was assigned mainly to the dangling bonds on the rest atoms. Finally, there was some evidence for tunneling from a lower-lying state, assigned to adatom backbonds, which would correspond to the state S_3. It is reasonable to assume that the origins of the various surface states on the Si(111)7×7-Ge and Si(111)5×5-Ge surfaces are the same as those for the surface states on the clean Si(111)7×7 surface.

The main changes in the surface electronic structure due to the presence of Ge atoms are a lowering in energy position of the rest-atom dangling-bond states by ~0.1 eV, a raising in energy position of the adatom back-bond states by ~0.25 eV (7×7-Ge) and ~0.45 eV (5×5-Ge), and a doubling of the total width of the empty adatom dangling-bond band. An interesting question is whether these changes are related to specific or to random positions of the Ge atoms. In this context, one can note that the results from a STM study of the Si(111)5×5-Ge surface suggested that Si and Ge atoms formed an ordered array of adatoms,[9] while a core-level photoemission study of the surface indicated that all Si adatoms were replaced by Ge atoms.[18] Considering the significant quantitative differences observed in the present study between the electronic properties of the Ge-covered surfaces and those of the clean surface, it is possible that a calculation of the electronic structure of a 2×2 model surface with Ge and/or Si adatoms and rest atoms would be sufficient to draw conclusions about the positions of the Ge atoms.

IV. SUMMARY

Using Auger-electron spectroscopy we have estimated the Ge content in the outer layers of Si(111)7×7-Ge and Si(111)5×5-Ge surfaces, either assuming a homogenous alloy within the probe depth or assuming a pure Ge

overlayer. The 5×5 reconstruction was observed on surfaces with a Ge content estimated to be 30–70 % of a homogenous alloy overlayer or 1.3–3.0 ML of pure Ge on top of the surface. A 7×7 reconstruction was observed on surfaces containing up to 24% of Ge, or, alternatively, up to 1.1 ML of Ge. With angle-resolved photoemission and inverse photoemission three occupied and one unoccupied surface-state bands have been identified for both surfaces, and the dispersions of these bands have been determined along the high-symmetry lines in the surface Brillouin zone. The electronic properties of the Ge-covered surfaces are found to be qualitatively similar to those of the clean Si(111)7×7 surface. The quantitative differences in the dispersions seem to correlate with the Ge content in the surfaces rather than with the surface periodicity, since concerning the dispersions, the 7×7-Ge surface is more similar to the 5×5-Ge surface than to the clean Si(111)7×7 surface.

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