PHYSICAL REVIEW B VOLUME 52, NUMBER 15 15 OCTOBER 1995-I

Clean and Cs-exposed Si(111)$\sqrt{3}\times\sqrt{3}$:B surface studied with high-resolution photoemission

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(Received 28 November 1994; revised manuscript received 2 June 1995)

Both the clean and Cs-exposed Si(111)$\sqrt{3}\times\sqrt{3}R\,30°$:B surfaces have been investigated by high-resolution photoemission. In the spectra from the Si $2p$ level, contributions were identified from the bulk, the adatoms plus the first layer, the second and $\frac{2}{3}$ ML of the third-layer atoms not binding to the B atoms, and, finally, the $\frac{1}{3}$ ML of third-layer atoms binding to the boron atoms. The interaction between the Cs atoms and the surface is found to be dependent on the coverage. At low coverages the geometric and electronic structure of the Si(111)$\sqrt{3}\times\sqrt{3}R\,30°$:B interface is only to a minor degree affected by the presence of Cs on the surface. At high coverage the Cs atoms react with the surface and alter the binding configuration of the Si adatoms.

I. INTRODUCTION

Due to their simple electronic structure alkali-metal (ns^1) adsorption on the Ge and Si surfaces is studied as a model system for the metal-semiconductor interaction. In these studies it is important to have a well-defined substrate surface. One example is the Si(111)$\sqrt{3}\times\sqrt{3}R\,30°$:B (Si$\sqrt{3}$:B for short) surface, which has been studied with a number of surface science techniques.[1-8] It has been shown that this surface is terminated by Si atoms in the $\sqrt{3}\times\sqrt{3}$ geometry. The boron atoms occupy the B-S_5 position in the second layer directly below the Si adatoms. Since boron has a valence of III, one electron is donated from the dangling bond of the Si adatom to the boron atom directly below. As a result the surface displays an unoccupied state of p_z type (dangling bond). Both the empty and the two filled back bond states associated with the Si adatoms have been identified experimentally by angle-resolved inverse and direct photoemission (KRIPES and ARPES).[5,8]

In the first core-level spectroscopy study of the clean Si$\sqrt{3}$:B it was shown by McLean, Terminello, and Himpsel that the Si $2p$ spectrum recorded at 130 eV was dominated by contributions from the overlayer and in order to account for the large intensity in the surface related component the whole of the top two layers had to be taken into account.[6] Later, Rowe, Wertheim, and Riffe showed that the Si $2p$ core level is composed of at least four components, one bulk and three surface related structures representing [in progressively higher binding energy (BE)] the adatoms, all the Si atoms in the first, second, and fourth layers, and the atoms in the third layer binding to the boron atoms.[7]

In a recent core-level study of K adsorption on the Si$\sqrt{3}$:B surface it was argued that the interaction between the metal and the surface is mainly of an ionic nature.[9] In this picture electrons are donated from the alkali-metal atom to an unoccupied state of the clean surface.[10] The partially filled band would then cross the Fermi level, rendering a metallic surface. However, in two recent ARPES studies of this surface no density of states was observed at the Fermi-level.[11,12] Instead a new state was observed with a binding energy of 0.7 eV and when probed in the Γ-M' direction, this state showed a dispersion of only 0.1 eV.[11,12] The lack of dispersion indicated a low overlap of this state parallel to the surface. Weitering *et al.* concluded that up to saturation coverage, correlation effects determine the electronic properties of the interface.[12]

In this paper results from a high-resolution photoemission study of the clean and Cs-covered surface are presented. The Si $2p$ data from the clean surface are decomposed into four components [in accordance with Rowe, Wetheim, and Riffe[7]]. The assignment of the fitted components is slightly different from those presented in Ref. 7 and it is proposed that they stem from (a) the bulk, (b) the $\frac{2}{3}$ ML of Si atoms in the second layer plus the $\frac{2}{3}$ ML of atom in the third layer not binding to the boron atom, (c) the adatoms plus the whole first layer, and (d) the 1/3-ML atom in the third layer binding directly to the boron atoms.

The interaction between the Cs atoms and the substrate was found to be different at high and low coverage. At low coverage only minor changes were observed in the valence band and the Si $2p$ and Cs $4d$ and B $1s$ core levels. This indicates a weak electronic interaction between the Cs atoms and the substrate at low coverage. At high coverage a new state developed in the valence band and the B $1s$ level became split into two components. A component to the low BE side in the Si $2p$ level displayed a fast intensity increase in this coverage region. Based on this experimental observation it is proposed that Cs

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reacts with the surface at high coverage and that the Cs atoms mediate the breaking of bonds between the first layer and the adatoms.

II. EXPERIMENTAL DETAILS

The photoemission studies were performed at beamline 22 at the MAXLAB Synchrontron Radiation Facility in Lund, Sweden. This beamline is equipped with a modified ZEISS SX-700 monochromator and a 200-mm 180° hemispherical energy analyzer.[13] A total-energy resolution of <0.1 eV was used for the Si 2*p* and Cs 4*d* levels, while the valence-band data and the B 1*s* level were recorded with a resolution of <0.2 eV. All spectra shown in this paper were recorded at normal emission relative to the surface plane. Fitting of the core-level data was performed using a nonlinear least-squares fitting procedure, utilizing spin-orbit (S-O) coupled doublets consisting of Voigt functions.[14]

Prior to insertion into the spectrometer the samples were implanted with B ions of 90-keV energy to a coverage of 5×10^{15} cm^{-2} (i.e., ≈ 6 ML), using a commercial process. Outgassing of the sample and preparation of the Si$\sqrt{3}$:B surface were performed *in situ* by resistive heating to 600 °C and 1050 °C, respectively.

Cesium was evaporated from well outgassed chromate dispensers (SAES Getters S.p.A.). During evaporation the pressure never exceeded 1×10^{-1} Torr and the base pressure was better than 8×10^{-11} Torr.

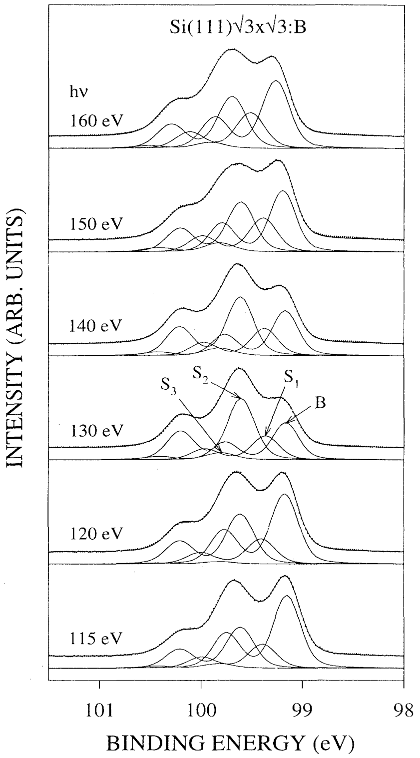

FIG. 1. The Si 2*p* level from the Si$\sqrt{3}$:B surface, recorded at various photon energies. The spectra are decomposed into one bulk (B) and three surface related components (S_1, S_2, and S_3).

III. RESULTS

A. The clean Si(111)$\sqrt{3}\times\sqrt{3}$:B surface

Depicted in Fig. 1 are Si 2*p* spectra from the clean Si$\sqrt{3}$:B surface, recorded at various photon energies. The spectra are decomposed into four components labeled B, S_1 S_2, and S_3. Fitting parameters and the BE of the resolved components from some 130-eV spectra are given in Table I. The relative intensities of the fitted components show a large dependence on the photon energy. Since the electron mean free path curve has a minimum at around 25–35 eV the spectra recorded with a photon energy of 130–140 eV ($E_{\rm kin}\sim 25$–35 eV, respectively) have the largest surface contributions and hence the smallest representation from the bulk. It is therefore clear that the component to lowest BE represents the bulk atoms and that the other components can be attributed to the surface. Since the S_3 component cannot be identified directly from the raw data, its absolute BE and intensity is determined with some uncertainty. It is noticeable that the BE of the bulk related component and the shift of the fitted components were independent of the photon energy, contrary to the observation made on less heavily doped samples.[6] Moreover it was found that repeated annealing cycles did not affect the core-level spectra. It is therefore concluded that the preparation used here gives a well-defined and stable surface.

B. Si(111)$\sqrt{3}\times\sqrt{3}$:B-Cs

For all metal coverages the surface displayed a $\sqrt{3}\times\sqrt{3}$ low-energy electron diffraction (LEED) pattern, which had a somewhat increased background after long deposition times. The development of the work function, measured by the onset of the secondary electrons, and the integrated intensity of the Cs 4*d* level as a function of deposition time, is shown in Fig. 2 (filled circles and triangles, respectively). As a guide for the eye a curve is fitted to each data set. Initially a linear relation is observed for both the changes in the work function ($\Delta\phi$) and the integrated intensity as a function of deposition time. A minimum in the work function is observed after 130–150 s and $\Delta\phi=-3.0$ eV and around this deposition time the Cs 4*d* intensity curve levels off. After longer deposition times both the work function and the coverage increase slightly.

Figure 3 displays the evolution of the Si 2*p* core level as a function of Cs coverage. The fitting parameters used in the decomposition process of the Si 2*p* and Cs 4*d* and B 1*s* core levels are given together with the BE for some selected spectra in Table I. The raw data show only minor changes in the shape below 60 s of Cs deposition but an intensity transfer from the high to the low BE part of the spectra is observed at high coverages.

A closer inspection of the decomposed components reveals that the bulk component moves to lower BE and in-

TABLE I. The BE of the bulk Si $2p_{3/2}$ components are given together with the energy shift of the other fitted components, the BE of the Cs $4d_{5/2}$ components and the B 1*s* level. The Gaussian width are given inside the parentheses appearing after the energy values. Lorentzian widths of 0.085, 0.17, and 0.17 eV were used for the Si 2*p*, Cs 4*d*, and B 1*s* levels, respectively.

$\mathrm{Si}2p_3$	BE and energy shifts (eV)		Relative intensity	Asymmetry index	$\mathrm{Cs}4d_{5/2}$	BE (eV)		Relative intensity	Asymmetry index	B1*s*	BE (eV)	Relative intensity
					Si(111)$\sqrt{3}\times\sqrt{3}$:B clean							
B	99.17	(0.27)	0.28							B_1	187.70(0.30)	1
S_1	0.20	(0.27)	0.18									
S_2	0.4	(0.27)	0.48									
S_3	0.65	(0.27)	0.06									
					Si(111)$\sqrt{3}\times\sqrt{3}$:B-Cs 45 s							
B	99.11	(0.28)	0.37		C_1	77.05	(0.72)	1		B_1	187.71(0.32)	1
S_1	0.28	(0.28)	0.18									
S_2	0.46	(0.28)	0.41									
S_3	0.68	(0.28)	0.01									
S_4	−0.38	(0.40)	0.03									
					Si(111)$\sqrt{3}\times\sqrt{3}$:B-Cs 150 s							
B	99.06	(0.32)	0.49	0.03	C_1	77.21	(0.69)	0.21	0.08	B_1	187.94(0.40)	0.86
S_1	0.34	(0.32)	0.24	0.03	C_2	76.74	(0.69)	0.79	0.08	B_2	186.83(0.04)	0.14
S_2	0.59	(0.32)	0.20	0.03								
S_4	−0.45	(0.37)	0.07	0.03								
					Si(111)$\sqrt{3}\times\sqrt{3}$:B-Cs 300 s							
B	98.97	(0.30)	0.51	0.09	C_1	77.22	(0.69)	0.10	0.19	B_1	187.89(0.40)	0.68
S_1	0.03	(0.30)	0.25	0.09	C_2	76.60	(0.69)	0.90	0.19	B_2	186.77(0.40)	0.32
S_2	0.54	(0.30)	0.15	0.09								
S_4	−0.44	(0.37)	0.09	0.09								

creases in intensity with coverage. Using the bulk component of the clean Si$\sqrt{3}$:B spectrum as a reference, BE shifts of −0.11 and −0.20 eV were measured after 150 and 300 s of metal deposition, respectively.

The relative intensity of the S_1 structure increases from 18% for the clean surface to 24% in the 150-s spec-

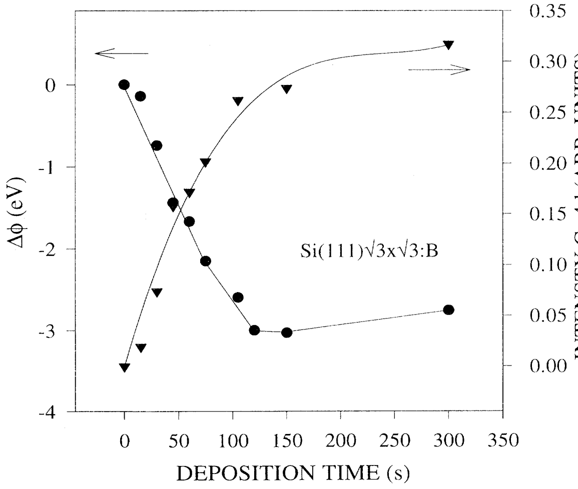

FIG. 2. The change in work function (circles and left axis) and the integrated intensity in the Cs 4*d* level (triangles and right axis) as a function of deposition times. As a guide to the eye each data set has been fitted to a curve.

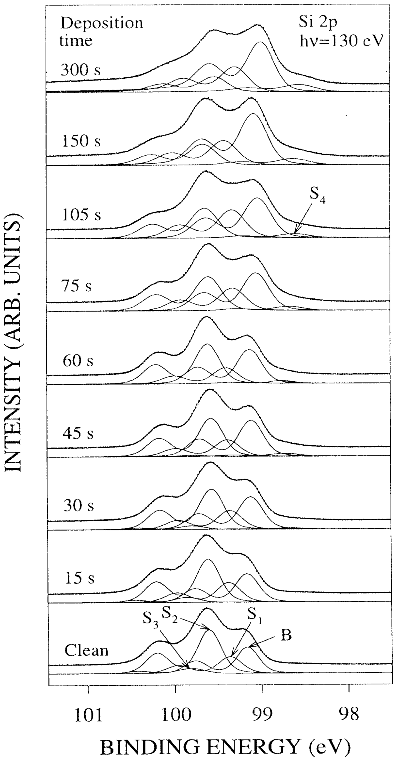

FIG. 3. Decomposed Si 2*p* data recorded at different Cs coverages with 130-eV photon energy.

trum and the relative intensity of the S_2 component decreases up to saturation almost linearly with coverage from 48% in the clean surface to 20% in the 150-s spectrum. Finally, the S_3 structure decreases rapidly in intensity with coverage and no spectral intensity can be detected in surfaces exposed to more than 45 s of Cs vapor.

The adsorption of Cs on the surface induces a new structure on the low-BE side of the bulk, labeled S_4 in Fig. 3. The intensity of the component is low up to the 75-s spectrum. Above 60 s the intensity of this component grows quickly with increasing coverage. A BE shift of -0.45 eV and a relative intensity of 7% and 9% is measured for this component in the Si $2p$ spectrum from the 150- and the 300-s surfaces, respectively. In order to obtain a high-quality fit a Doniach-Šunjić asymmetry index had to be imposed when fitting the 150- and 300-s spectra.

At low coverage the Cs $4d$ level can be decomposed into one component, labeled C_1 in Fig. 4. After 60 s of metal deposition a new structure, C_2 appears at low BE. At higher coverages the C_2 component displays the fastest intensity growth and it dominates the spectrum from the saturated surface. Similar to the fit of the Si $2p$ spectra, an asymmetry index had to be used when fitting the 150- and 300-s spectra.

In Fig. 5 the development of the valence band is displayed as a function of coverage. The most interesting changes in the spectra occur close to the Fermi level.

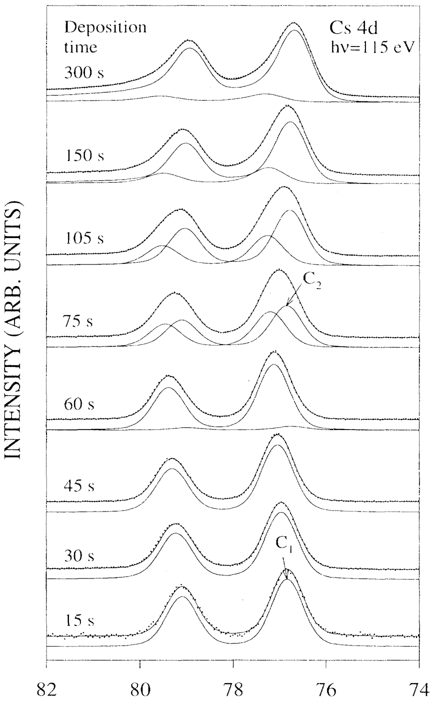

FIG. 4. The evolution of the Cs $4d$ level as a function of Cs exposure time.

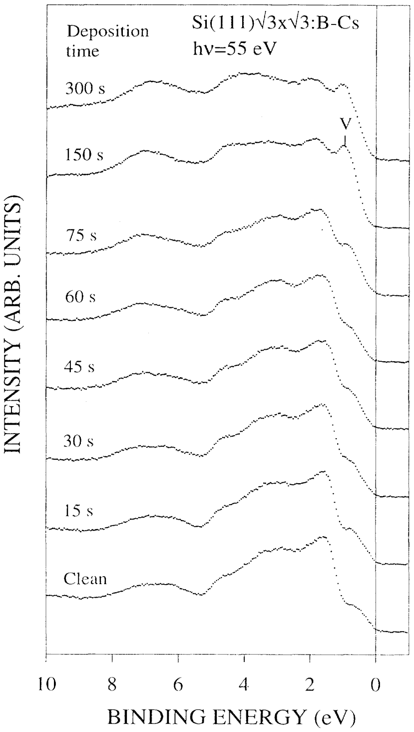

FIG. 5. The development of the valence band as a function of Cs coverage.

The BE of the bulk level in the Si $2p$ level from the clean surface is 99.17 eV. This means that the energy difference between the Fermi level and the valence band maxima is 0.4 eV.[15] In the valence-band spectrum from the clean surface, the top of the valence band can be seen 0.4–0.5 eV below the Fermi level. The intensity of the valence-band maximum decreases up to the Fermi level and no density of states can be observed at the Fermi level. It is also possible that some intensity at a BE of 0.3–0.2 eV below the Fermi level could spring from defect states observed on the clean surface. In a previous study these defects were attributed to Si adatoms in a $\sqrt{3}\times\sqrt{3}$ geometry but without a boron atom in the B-S_5 geometry.[8] Since prolonged annealing cycles did only have a minor impact on the valence-band and Si $2p$ spectra, we estimate the defect density to be low on the studied surfaces.

It should be noted that no spectral intensity is observed at the Fermi level at any coverages. A new state, labeled V, becomes visible in the 75-s spectra. For high coverages it shows a swift intensity increase.

The recorded B $1s$ spectra are depicted for various metal coverages in Fig. 6. Up to 150 s the B $1s$ level is composed of one component. Up to 60 s of Cs deposition the BE of this component is independent of the coverage. At higher coverages the structure moves to higher BE. In the 150-s spectrum a new structure becomes visible, and a BE shift of 1.2 eV is measured between the two structures. The intensity of the low BE component increases with coverage. Added in the top part of Fig. 6 is a spec-

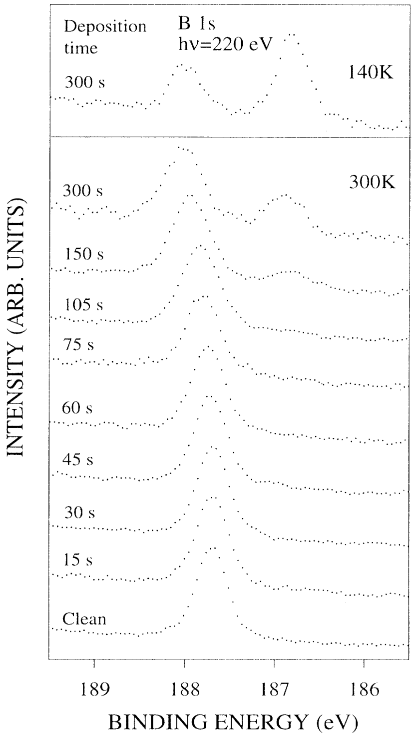

FIG. 6. The B 1*s* core levels recorded at different Cs coverages at room temperature. The uppermost spectrum was recorded after depositing Cs on a sample held at 140 K.

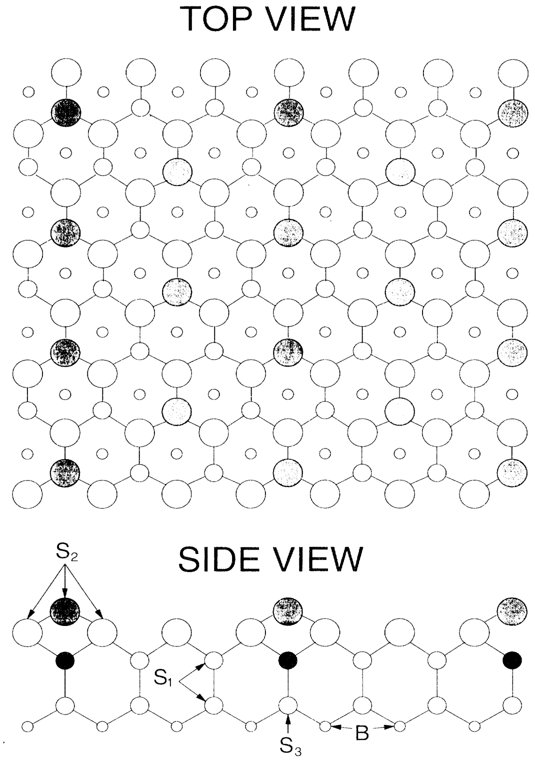

FIG. 7. A model of the Si$\sqrt{3}$:B surface. Added in the figure is the notation used for the corresponding components in the Si 2*p* level. The large filled circles represent the adatoms and the small filled circles represent the boron atoms.

trum recorded from a surface exposed to 300 s of Cs at low temperature (140 K). The Cs coverage in this spectrum is 10% higher than in the corresponding spectrum recorded from a sample held at room temperature.

IV. DISCUSSION

Depicted in Fig. 7 is a schematic drawing of the Si$\sqrt{3}$:B surface. The surface region contains the following groups of Si atoms: the adatoms, the first-layer atoms, the $\frac{2}{3}$ ML of second-layer atoms, the $\frac{2}{3}$-ML third-layer atoms not binding to the boron atom, and the $\frac{1}{3}$ ML of third-layer binding to the boron atoms. All atoms below the third layer are attributed to the bulk. Since the boron atom is more electronegative than the Si atom (2.04 vs 1.90) (Ref. 16) an energy shift to higher BE can be expected for the Si atoms binding to the boron atoms.[17] The S_2 component in the Si 2*p* level showed the highest intensity in the 130-eV spectra. Morar *et al.*[18] have shown that the mean free path curve for the Si 2*p* photoelectrons has a minimum around a kinetic energy of 25 eV, which for Si 2*p* corresponds to a photon energy of about 130 eV. It is thus reasonable to assign the emissions from the first layer to the S_2 component.

In a recent core-level study of the Si(111)7×7 surface the contribution from the adatoms was identified shifted 0.5 eV to higher BE relative to the bulk.[19,20] Since the adatoms on the Si(111)7×7 surface have half-filled dangling bonds and the adatoms on the Si$\sqrt{3}$:B surfaces have empty dangling bonds, in a charge-transfer model (neglecting final-states effects) it would be expected that the latter should have a larger BE shift. This would make the S_3 structure a feasible candidate for the adatom contribution. However, the intensity of this structure is too small to comprise the emission from the adatoms. We instead suggest that the adatom contribution is included in the S_2 component. It is possible that the S_3 structure stems from atoms in the third-layer binding to the boron atoms and shifted due to the strain induced by the smaller bond length of the boron atom.[7] On the other hand, the intensity of the S_3 component decreased rapidly after Cs adsorption. The low intensity of this component in combination with the fact that it is not possible to identify it directly from the raw data makes the identification of this structure somewhat uncertain.

The S_1 structure was only to a minor degree affected by the Cs adsorption, which indicates that this component originates from atoms in a subsurface position. In order to rationalize the intensity in this component, contributions from both the second layer and the $\frac{2}{3}$ ML of atoms in the third layer not binding to the boron atoms has to be included.

After exposing the surface to Cs the LEED pattern still exhibited a distinct $\sqrt{3}\times\sqrt{3}$ at low coverage that became less distinct at high coverages. In a previous study of the Si$\sqrt{3}$:B-K surface a faint 2×2 pattern was observed at high coverage.[9] In the present study no sign of any extra LEED spots could be found at any of the investigated coverages.

A closer inspection of the Si 2*p*, Cs 4*d*, valence band and the B 1*s* levels in the 0–60-s coverage region reveals only minor changes in the shape and the BE of the embodied structures. Above 60 s several changes took place: the Si 2*p* component to lower BE (S_4) displayed a swift intensity growth with the coverage, a second component became visible in the Cs 4*d* level, a new structure became clearly visible at ~1 eV below the Fermi level in the valence band, and the B 1*s* level started to move to lower BE. After 150 s of Cs deposition the B 1*s* level became split into two structures shifted 1.2 eV apart. The adsorption process can thus be divided into a low-coverage region (0–60 s of metal deposition) and a high-coverage region (75 s of metal deposition and above).

Since only minor changes were observed in the spectra in the low-coverage regime it is reasonable to assume that the interaction between the surface and the adsorbate is weak. By a weak interaction we mean that no large charge-transfer process has occurred and that the basic electronic and geometric structure of the Si$\sqrt{3}$:B surface is preserved. Ma *et al.* have performed x-ray photoadsorption (XAS) and core-level spectroscopy measurements on the Si$\sqrt{3}$:B-K surface.[9] At low coverage the prespike (transition from the B 1*s* to the unoccupied surface state) in the XAS data from the B *K* edge showed no apparent changes.[9] At higher coverage an intensity attenuation of the prespike follows the intensity decrease of the B 1*s* level.[9] This indicates that the reaction path might be similar for K and Cs on the Si$\sqrt{3}$:B surface.

No density of states was observed at the Fermi level in the valence-band spectra at any coverages. A similar observation has been made for the Si$\sqrt{3}$:B-K surface.[11,12] On the clean Si$\sqrt{3}$:B surface the empty state has an energy minimum that is 0.8 eV above the Fermi level.[5,8] A partial filling of this state by K has not been observed.[11,12] The absence of spectral changes and the persistence of the surface geometry therefore points to that the Cs valence electron is mainly localized to the metal atoms at low coverages.

At low coverages the Cs 4*d* level was composed of one component (C_1). In the 60-s spectra a new structure C_2 became visible. This structure displayed a fast intensity increase with coverage. As can be seen in Fig. 2 the coverage after 60 s of Cs deposition is $\sim\frac{2}{3}$ of the value obtained in the 150-s spectra where the C_2 structure dominates. The dramatic intensity redistribution occurring after the surface is exposed to more than 60 s of the Cs 4*d* level can therefore not be explained by assuming that C_1 and C_2 represents two geometrically different sites. Instead it is more likely that the C_1 and C_2 components can be associated with patches on the surface with different Cs-Cs distances so that C_2 represents a more dense Cs overlayer.

At high coverage the Cs reacts with the surface and the reaction can be followed by the appearance of a new component in the B 1*s* spectra and the increase in the low BE component (S_4) in the Si 2*p* level. The energy shift of the S_4 component (−0.45 eV) is of the same order as the shift observed when adsorbing Cs on the Si(111)7×7(−0.57 eV).[21]

The S_2 component was identified as emission from both the adatoms and the atoms in the first layer. The relative intensity of this structure was 48%, 20%, and 15% in the spectra from the clean, 150- and 300-s spectra, respectively. Part of the spectral intensity in the S_2 structure is transferred to the S_4 component. The decrease in intensity cannot be fully explained in terms of attenuation due to the Cs overlayer. Instead a feasible explanation for the intensity decrease in the S_2 structure is that at high coverage the Cs reacts with the surface and mediates a breaking of the bonds to the adatoms. This will then alter the BE of the surrounding first-layer atoms and as a consequence the relative intensity of the S_2 component is weakened.

In the B 1*s* level a new component, shifted −1.2 eV to lower BE, becomes visible in the 150-s spectra. As can be seen in Fig. 6 the intensity of the low-BE component is strongly dependent on the Cs coverage. A similar observation of the development of the B 1*s* level as a function of coverage has been made by Ma *et al.*[9] The extra component in the B 1*s* level can be associated with reacted parts on the surface. A reaction between the Cs atoms and the surface would involve breaking of bonds. Due to the geometry of the surface the adatoms are the atoms that are most likely to react. Moreover it has been shown that Li and K can mediate the removal of the adatoms on the Ge(111)*c*(2×8) surface[22] and that Li reacts with the chemically stable Si(111)7×7 surface by removal of the adatoms.[23] It is thus likely that at high metal coverages, the Cs atoms can also mediate the breaking of bonds to the adatoms on the Si$\sqrt{3}$:B surface. The resulting charge balance after a reaction has occurred on the surface is delicate. The valence-band spectra reveal no density of states at the Fermi level, which indicates that we do not have any, or only a very low concentration of, half-filled dangling bonds on the surface. After breaking a bond to an adatom the excess charge is dominated to the B atom, which changes its valence, as shown by the appearance of the low-BE component in the B 1*s* spectra as arising from boron atoms with a higher valence number.

In order to increase the sticking coefficient of the surface a sample held at low temperatures was exposed to Cs for 300 s. This resulted in a 10% increase of the amount of Cs on the surface relative to the room-temperature deposition and a drastic increase of the low-BE component in the B 1*s* level. This shows that the reaction is not kinetically controlled, instead it is found that the reaction is highly dependent on the amount of Cs on the surface. Similar observations have been made on the Si(111)-Li, Ge(111)-Li, and Ge(111)-K (Refs. 21 and 22) adsorption systems.

The work-function curve (Fig. 2) shows a minimum at $\Delta\phi - 3.0$ eV and a deposition time around 130–150 s. At this coverage and above both the Si 2*p* and Cs 4*d* levels displayed an asymmetric line profile. Since no density of states was observed at the Fermi level in the valence-band spectra it is unlikely that the asymmetries can be connected with the shielding of the core levels. Instead it is possible that the asymmetry can be connected with the creation of a free carrier plasmon as has been observed for the clean surface.[24]

V. CONCLUSION

In summary, the clean and Cs-exposed surfaces have been investigated by high-resolution photoemission. The Si 2*p* spectra from the clean surface could be fitted with four components representing the bulk, the adatoms plus the first layer, 2/3-ML second- and third-layer atoms not binding directly to the boron atoms, and finally the atoms in the third layer binding to the boron atoms.

It was found that the Cs adsorption process can be divided into a low- and a high-coverage region. In the low-coverage regime the interaction between the Cs atoms and the surface is weak. Moreover, it is proposed that the Cs 6*s* electron is mainly localized to the Cs atom in this regime.

At high coverage significant changes are observed in the probed core levels and the valence band as a result of a reaction between the Cs atoms and the surface. The evidences are as follows: the Si 2*p* S_2 component became strongly attenuated, the S_4 component in the Si 2*p* level showed a fast intensity increase with coverage, a new state was observed in the valence band, and a new component appeared in the B 1*s* level.

ACKNOWLEDGMENTS

The assistance of the Max-lab staff is gratefully acknowledged. This work was supported by the Swedish Natural Science Research Council (NFR) and the Swedish Research Council for Engineering Science (TFR).

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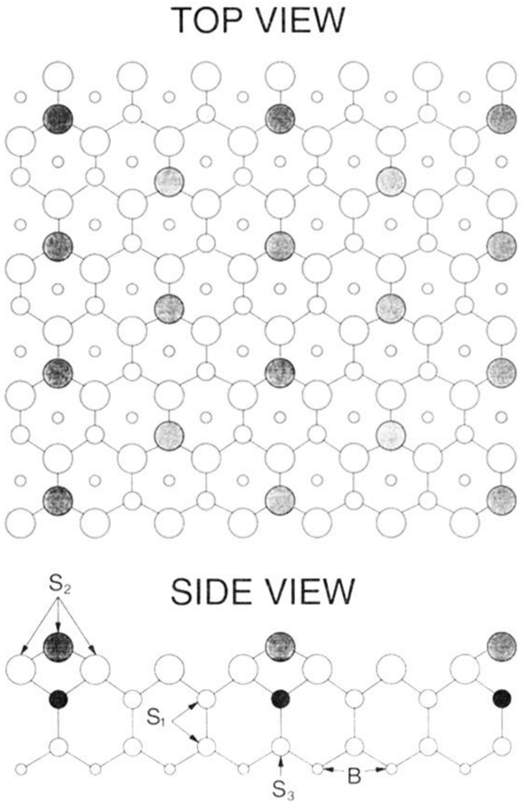

FIG. 7. A model of the Si$\sqrt{3}$:B surface. Added in the figure is the notation used for the corresponding components in the Si $2p$ level. The large filled circles represent the adatoms and the small filled circles represent the boron atoms.