

Atomic origin of the surface components in the high-resolution Si 2p core level spectrum of Si (110) $\sqrt{8\times 2}$

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2001 J. Phys.: Condens. Matter 13 6609

(<http://iopscience.iop.org/0953-8984/13/31/302>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.226

The article was downloaded on 16/05/2010 at 14:02

Please note that [terms and conditions apply](#).

Atomic origin of the surface components in the high-resolution Si 2p core level spectrum of Si (110) '8 × 2'

N Safta

Département de Physique Faculté des Sciences, Avenue de l'environnement, 5000 Monastir, Tunisia

Received 5 February 2001, in final form 17 May 2001

Published 19 July 2001

Online at stacks.iop.org/JPhysCM/13/6609

Abstract

An analysis, based on the results for Si(111) 7×7 , is performed about a well resolved Si 2p core level spectrum from the clean Si (110) '8 × 2' surface measured with synchrotron radiation. We identify the contributions from the constitutive entities of the '8 × 2' superstructure. We also obtain by quantitative analysis the number of atoms of such an entity per one unit cell of the '8 × 2' surface.

1. Introduction

In the early years, few studies confirmed that the clean Si (110) face is characterized by only one superstructure, '16 × 2' [1–5], and some geometrical models have been proposed to explain the experimental data [6, 7]. A theoretical study suggests that building elements might be involved, similar to those in Si (111) '7 × 7' reconstruction, especially adatoms, rest atoms and vacancies. The first confirmation, which has come from photoemission yield spectra, suggested that the reconstruction should also involve a few consecutive atomic planes in depth [1]. The second confirmation, which has come from a study of angle-resolved ultraviolet photoemission (ARUPS) [8], showed the electronic properties of the surface state bands to be very similar to those of Si (111) '7 × 7'.

In addition, core level photoemission has been largely used to assign different surface contributions to the respective entities of the different reconstructions. This is certainly due to the technical developments that have permitted high-resolution photoelectron spectroscopy studies to be performed with synchrotron radiation in the soft X-regime. Then, well resolved Si 2p core level spectra using photon energies of around 150 eV with experimental resolutions better than 80 meV and an emission angle of around 55° have been obtained [9–11]. This permits us to link the causal relationships between the geometric and electronic structures of surfaces and interfaces.

In a previous work [12] we have described and studied the Si (110) 8×2 superstructure, which is better ordered than Si (110) '16 × 2'. We have confirmed, by core level photoemission, that the Si (110) '8 × 2' surface involves a similar local structure, especially adatoms, rest atoms,

dimer atoms and pedestal atoms, as the well known DAS model [13] for the Si (111) '7 × 7' reconstruction. However, until now, never has a study dealt with the assignment of the surface components of the Si 2p core level to the different entities of the '8 × 2' superstructure.

This constitutes one of the subjects of the present paper. In addition, using quantitative analysis based on the intensity ratio of Si 2p components, we propose a number of atoms of such an entity per one '8 × 2' surface unit cell. All our analyses are related to the decomposition of the Si 2p core level spectra from the closely related Si (111) '7 × 7' superstructure proposed in [14]. The results given in [15] are also taken into account.

2. Si 2p core level analysis

In the first step, we analyse figure 1, taken from [14], which shows the Si 2p spectra for the prototypical Si (111) '7 × 7' surface acquired firstly at $h\nu = 140$ eV, $T = 300$ K and an emission angle θ_e of 60° , and secondly, $h\nu = 150$ eV, $T = 300$ K and an emission angle θ_e equal to 0° . S_5^* shifts by -0.7 eV (i.e. to a lower binding energy than the bulk line), which corresponds to the rest atoms, S_2^* shifted 0.5 eV to higher binding energy springs from adatoms emission, while S_3^* at high binding energy (0.24 eV) originates from pedestal atoms. S_4^* at -0.1 eV is associated either with the dimer atoms or to later atoms in one half of the unit cell [15]. Finally, S_1^* reflects a shakeup structure or a defect.

In the second step, we present the surface unit cell of Si (110) '8 × 2' displayed in figure 2. The unit vectors are given as:

$$A_1 = \frac{17}{2}b - \frac{1}{2}b \quad \text{and} \quad B_1 = -2a + 2b.$$

In the third step, we present the decomposed spectra of Si (110) '8 × 2' given by [12] (figure 3). The same decomposition procedure as in [14] has been followed for all the spectra which means that comparisons are valid: in addition to the spin-orbit splitting, a value of 0.605 eV was assumed, and the width of the lorentzian curve showing the natural width of the peaks was taken to be 35 meV. The values of the various parameters used in the decomposition are given in table 1. The origin of the energies is taken at the Si 2p $B_{3/2}$ of the bulk component B , and increasing binding energies are taken as positive. This consistent analysis reveals at least five surface components. The assignments of surface contributions is based on their energetic shift values relative to the bulk line compared with those of the Si (111) '7 × 7' superstructure.

For the Si (111) '7 × 7' surface, the strongest surface peak S_3^* at 0.24 eV was attributed to the pedestal atoms. For the same reason we can assign S_3 situated at 0.15 eV from the origin to the corresponding pedestal atoms; their number will be discussed later. The S_1 shift of 0.755 eV to a lower binding energy is, therefore, as for S_5^* in the case of Si (111) '7 × 7', attributed to the rest atoms. The energetic shift value of the S_4 component is 0.40 eV to a higher binding energy. Comparison with the shift value of S_2^* in the case of the Si (111) '7 × 7' indeed confirms the adatom origin of this contribution. The shift value of S_2 (0.2 eV to a lower binding energy) is practically the same as the shift of S_3^* , corresponding to dimer atoms contribution. We will show later that S_2 must be assigned, in addition to the dimer, to another atom configuration. Finally, the shift of S_5 is equal to 0.892 eV. This value is equal to the case of S_1^* for Si (111) '7 × 7', assigned to a shakeup structure or to defects. We will assign the shift of S_5 to defects.

Now, we will examine the constituent intensities. For this purpose, we must consider the Si (100) '8 × 2' spectrum shown in figure 3(c) and that of Si (111) '7 × 7' in figure 1(a) because they were obtained under the same experimental conditions ($h\nu = 140$ – 141 eV, $\theta_e = 0^\circ$ and $T = 300$ K). Our analysis is based on the relationship existing between the intensities ratio of the surface peak of a given configuration with regard to that of the bulk ($R_{IS^*} = I_S/I_B$),

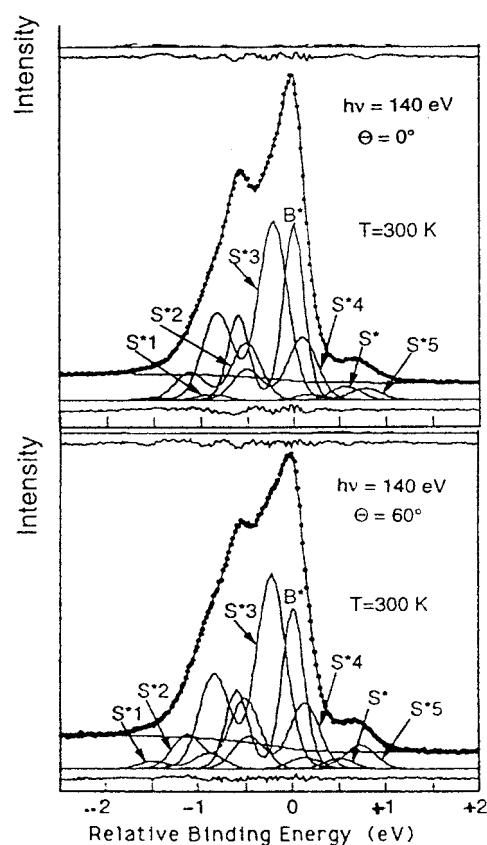


Figure 1. Si 2p spectra for the prototypical Si (111) '7 × 7' surface.

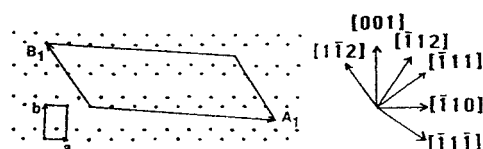


Figure 2. A unit cell of the Si (110) '8 × 2' surface.

and the ratio corresponding to the number of surface atoms compared with that of the bulk, relative to a single reconstructive cell (7×7) ($R_{nS^*} = n_S/n_B$). As a rough guide, in the case of adatoms, R_{IS^*} is equal to 0.32 while $R_{nS^*} = 0.24$ (12/49). So we can deduce by a simple 'rule of three' that in the case of adatoms, if $R_{IS^*} = 1$ so $R_{nS^*} = 0.75$ (0.24/0.32). The same reasoning for the other surface configurations gives different results, as indicated in table 2.

Since the local atomic arrangement of the surface is similar for Si (111) and Si (110), the same relationship between R_{nS^*} and R_{IS^*} for a given surface configuration can be used in the case of Si (110) '8 × 2'. So the first step, and for every surface configuration, is to determine the intensities ratio of the surface peak with regard to that of the bulk (R_{IS}). Then we must find the corresponding ratio of the number of surface atoms to that of the bulk R_{nS^*} . Finally, the number of surface atoms is deduced by using the relation $n_S = R_{nS^*}n_B = 32$ ($8 \times 2 \times 2$) for a cell 8×2 .

Figure 3(c) shows that $R_{IS1} = 0.09$ which gives $R_{nS1} = 0.14$. So, $n_S \approx 3.84$, and n_{S1} relative to rest atoms is approximately equal to 4. Concerning S_2 , with $R_{IS2} = 0.63$, $R_{nS2} = 0.87$ so $n_{S2} \approx 28$. As for S_3 , from $R_{IS3} = 0.91$, we can deduce that $R_{nS3} = 0.67$ and, consequently, n_{S3} associated to pedestal atoms is practically equal to 21. By simple calculation, we can obtain R_{nS4} and n_{S4} relative to adatoms as being equal to 14.

However, note that the number of adatoms necessitates 42 pedestal atoms. Obtaining by

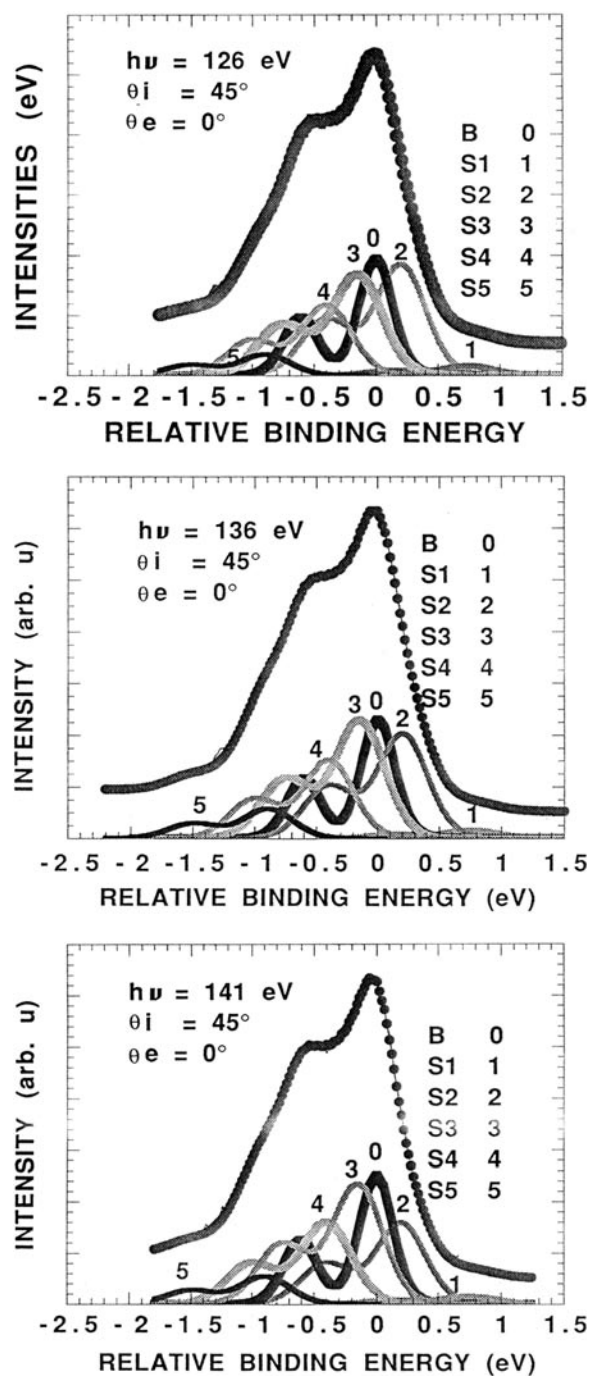


Figure 3. Si 2p spectra for the Si (110) '8 × 2' surface.

calculation only 24 pedestal atoms, let us assume that the number of real 'true' adatoms would be seven, while the other seven represent configurations which resemble adatoms. The S_2

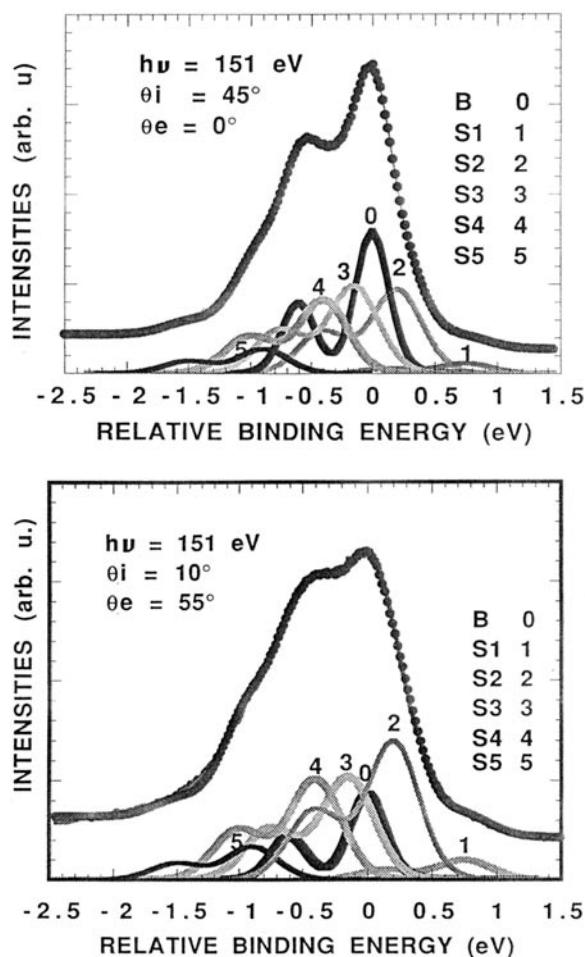


Figure 3. (Continued)

component, associated to 28 atoms, is then assigned to 21 configurations similar to pedestal atoms and seven dimer atoms.

The complexity of Si (110), also related to the ideal surface structure, leads to the new type of atoms corresponding to defects: seven configurations very similar to adatoms and 21 configurations like pedestal atoms.

3. Conclusion

To summarize, we have unambiguously identified the contribution of the building entities of the Si (110) '8 × 2' reconstruction: the rest atoms at -0.755 eV binding energy, the adatoms at $+0.400$ eV, and the pedestal atoms at 0.150 eV, as well as the dimer atoms and the new type of atoms at -0.200 eV. We have also obtained the number of atoms of these entities per one perfect '8 × 2' surface unit cell: 21 pedestal atoms, four rest atoms, seven dimer atoms and seven adatoms. We have thus opened up new routes for proposing an accepted model for the Si (110) '8 × 2' superstructure, similar to the known DAS model proposed for Si (111) '7 × 7'.

Table 1. Fitting parameters for the Si 2p spectrum.

Si 2p	$h\nu = 151 \text{ eV}$ $\theta_e = 55^\circ$
Branching ratio	$B = 0.5$ $S_1 = 0.50$ $S_2 = 0.50$ $S_3 = 0.50$ $S_4 = 0.50$ $S_5 = 0.50$
Gaussian width (eV)	$B = 0.30$ $S_1 = 0.45$ $S_2 = 0.45$ $S_3 = 0.45$ $S_4 = 0.45$ $S_5 = 0.45$
Core level shift (eV)	$B = 0$ $S_1 = -0.755$ $S_2 = -0.200$ $S_3 = +0.150$ $S_4 = +0.400$ $S_5 = +0.892$

Table 2. Relationship between R_{IS^*} and R_{nS^*} for different surface configurations.

	R_{IS^*}	R_{nS^*}	$R_{n_1^*}$ corresponding to $R_{IS^*=1}$
S_1^*	0.05		
S_2^*	0.32	0.24	0.75
S_3^*	1.02	0.73	0.74
S_4^*	0.36	0.50	1.38
S_5^*	0.06	0.12	2

References

- [1] Safta N, Lacharme J-P and Sébene C A 1993 *Surf. Sci.* **287/288** 312
- [2] Ichinowa T, Ampo H, Miura S and Tumura A 1993 *Phys. Rev. B* **31** 5183
- [3] Yamamoto Y, Ino S and Ichikawa T 1986 *Japan. J. Appl. Phys.* **25** L331
- [4] van Loenen E J, Dijkkamp D and Hoeven A J 1988 *J. Microsc.* **152** 487
- [5] Yamamoto Y, Shin-ichi Kitamura and Iwatsuki M 1992 *J. Appl. Phys.* **31** L635
- [6] Nesterenko B and Shkrebtii A I 1989 *Surf. Sci.* **213** 309
- [7] Shkrebtii A I, Bertoni C M, Del Sole R and Nesterenko B 1990 *Surf. Sci.* **239** 227
- [8] Cricenti A, Perfetti P, Nesterenko B, Le Lay G and Sebenne C 1996 *J. Vac. Sci. Technol. A* **14** 2248
- [9] Landemark E, Karlsson C J, Chao Y C and Uhrberg R I G 1992 *Phys. Rev. Lett.* **69** 1588
- [10] La Lay G, Aristov V Yu and Fontaine M 1994 *J. Physique* **IV** 213
- [11] Cicienti A, Ottaviani C, Comicioli C, Perfetti P and Le Lay G 1998 *Phys. Rev. B* **58** 7086
- [12] Safta N, Lacharme J P, Cricenti A, Taleb-Ibrahimi A, Indlekofer, Aristov V, Sébenne C A, Le Lay G and Nesterrnko B 1995 *Nucl. Instrum. Methods Phys. Res. B* **97** 372
Safta N 1994 *Thèse* l'Université Paris 7, Paris
- [13] Takayanagy K, Tanishiro Y, Takahashi M and Takahashi S 1985 *J. Vac. Sci. Technol. A* **3** 1502
- [14] Le Lay G, Gothelid M, Grehk M T, Björkquist M, Karlsson U O and Aristov V Yu 1994 *Phys. Rev. B* **50** 14 277
- [15] Le Lay G, Cricenti A, Ottaviani C, Hakansson C, Perfetti P and Prince K C 1998 *J. Electron Spectrosc. Related Phenom.* **88-91** 711