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Room temperature Si(001)-(2 × 1) reconstruction solved by X-ray diffraction

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Abstract

X-ray diffraction has been used to characterize the room-temperature atomic structure of the clean Si(001)-(2 × 1) reconstruction. Intensities of 276 half-integer order reflections have been measured and, after considering the symmetry of the system, they reduced to 44. Different models have been used to try to fit the experimental data. The best fit structure clearly indicates the presence of asymmetric dimers (bond length 0.267 nm and tilt angle 20°) with a disordered buckling direction. Atomic relaxations down to the sixth layer have been determined. From the analysis of the Si–Si bond distances we deduce that this (2 × 1) structure is likely to be a disordered version of a higher-order reconstruction, p(2 × 2) or c(4 × 2). © 1997 Elsevier Science B.V. All rights reserved.

Keywords: Silicon; Surface relaxation and reconstruction; X-ray scattering, diffraction, and reflection

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1. Introduction

The structures of the (2 × 1) reconstruction of the (001) surfaces of silicon and germanium have been extensively studied in order to determine the geometrical arrangements of the atoms and their electronic properties. Although the formation of dimers as the principal feature of the reconstructed surface is not in any doubt, there is still some controversy about their symmetry. Room-temperature scanning tunneling microscopy (STM) topographies [1] of the Si(001)-(2 × 1) surface show the presence of both symmetric and asymmetric dimers, the latter being observed near surface defects. Similar STM images on defect-free Si(001) surfaces [2] indicate the presence of symmetric dimers. A recent low-temperature STM study [3] clearly shows the presence of p(2 × 2) and c(4 × 2) buckled dimer domains which increase in number by cooling down to 120 K, suggesting that at room temperature, dimers rapidly switch their orientation, leading to a time-averaged (2 × 1) symmetric appearance.

Earlier energy minimization calculations [4] showed that the buckled dimer geometry is more stable and gives surface electronic bands in good agreement with photoemission data. However, more recent total-energy calculations [5] show contradictory results indicating that, at room temperature, the two models have small differences in energy. Angle-resolved ultraviolet photoelectron spectroscopy (ARUPS) results [6] also seem to confirm this, being compatible with either the symmetric or asymmetric dimer model. The pres-

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ence of asymmetric dimers in a large temperature range, from 40 to 310 K, was also recently proposed on the basis of microscopic calculation of the optical properties of the Si(001) surface [7]. Calculations based on the asymmetric model [8] found that the (2×1) reconstruction is not the most stable, and that higher-order reconstructions should occur. They also predicted an order–disorder phase transition which would cause the disappearance of higher-order diffraction peaks in a low-energy electron diffraction (LEED) pattern at about 250 K. In fact, the transition from a $c(4 \times 2)$ to a (2×1) reconstruction was observed by LEED measurements to occur at 200 K [9]. Core-level spectroscopy studies [10] on the clean Si(001) surface have shown a close similarity between the spectra obtained at low temperature for the $c(4 \times 2)$ reconstructions and those measured at room temperature for the (2×1) reconstruction. Moreover, underlying layers influence the observed spectral lines, indicating that the reconstruction induces a subsurface layer relaxation. These results support the picture of a $c(4 \times 2)$ (or $p(2 \times 2)$) to (2×1) phase transition during a loss of long-range order among the buckling dimer directions [11].

A previous X-ray diffraction study of this reconstructed surface [12] could not easily distinguish between symmetric and asymmetric dimers because of the lack of out-of-plane measurements, but indirectly suggested the presence of asymmetric dimers forming an angle of 7.4° with the surface. The presence of asymmetrical dimers was instead clearly indicated by both in-plane and out-of-plane X-ray diffraction measurements performed on the Ge(001)-(2×1) reconstructed surfaces [13], assuming a disordered model involving far-reaching subsurface relaxations.

In order to determine the dimer geometry and the relaxation of the inner layer atoms in Si(001)-(2×1) at room temperature, we have measured the intensity of fractional-order peaks as a function of the perpendicular momentum transfer q_z up to $q_z = 1.5\ c^*$, where $c^* = 1/a_3$ is the vertical reciprocal lattice unit.

2. Experimental

The experiment was performed on beam line X16A at the National Synchrotron Light Source of the Brookhaven National Laboratory. Radiation from a bending magnet was focused by a toroidal Pt-coated mirror and monochromatized to a wavelength of 0.15 nm by an Si(111) double-crystal monochromator. The incident beam was collimated to a dimension of 2.0 mm × 0.5 mm by tungsten slits. The scattered radiation was collimated by two slits of 4.0 mm in width and was collected by a position-sensitive detector.

Silicon samples (2.5 cm long, 0.6 cm wide) were cleaned by acid etching and then mounted inside a UHV chamber coupled to a five-circle diffractometer [14]. They were annealed using the following procedure: (i) slow heating up to 800°C, (ii) hold at 800°C for 1 h, (iii) flash at 1000°C for 30 s, (iv) hold at 800°C for 45 min, (v) slow cooling down to room temperature. During all of the above procedure the pressure was never higher than 1×10^{-7} Torr. The base pressure during the whole experiment was 1×10^{-10} Torr. In this way we were able to obtain (2×1) reconstructed surfaces, whose fractional order peaks had about the same full width at half maximum (FWHM) as the crystal truncation rods [15]. This implies a large coherent domain size. To determine the domain size of the reconstruction, a q-scan (or a ϑ–2ϑ scan) is necessary. We have not performed this kind of scan, but a rough estimation can still be done assuming that the peak width along the Φ scan is the same of the value measured along the q-scan. Under this approximation, and considering that the incident photon energy and the FWHM are 8 keV and 0.15°, we calculate a domain size of about 250 nm (Fig. 1).

The sample surface was aligned using a laser beam, while crystallographic alignment was achieved by determining the positions of two out-of-plane bulk Bragg reflections.

In order to simplify data collection, we used the following primitive real-space lattice with respect to the conventional fcc lattice

$$\boldsymbol{a}_1 = \tfrac{1}{2}\,[110]_{\mathrm{fcc}},$$

$$\boldsymbol{a}_2 = \tfrac{1}{2}[\bar{1}10]_{\mathrm{fcc}}, \qquad \boldsymbol{a}_3 = [001]_{\mathrm{fcc}}, \tag{1}$$

obtaining the following lattice dimensions:

$$|\boldsymbol{a}_1| = |\boldsymbol{a}_2| = \frac{a_0}{\sqrt{2}}, \qquad |\boldsymbol{a}_3| = a_0, \tag{2}$$

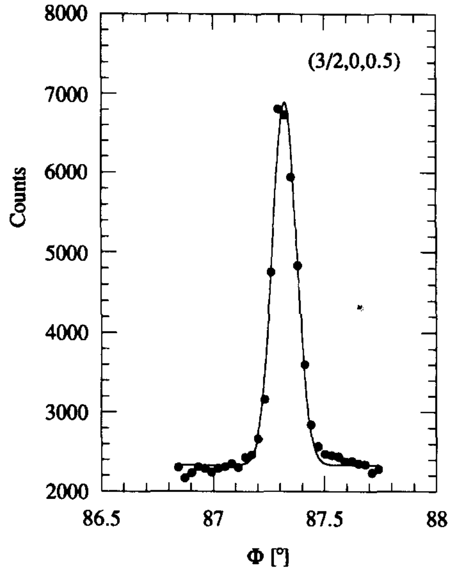

Fig. 1. Φ scan of one of the fractional order peaks. The line is a Gaussian fit through the experimental data. From the peak width we can calculate coherent domain dimensions of about 250 nm.

where a_0 is the silicon bulk lattice constant (0.543 nm).

The scan geometry was chosen in order to have equal incident and exit angles of the beams with respect to the sample surface. The integrated intensities were measured by ω scans and normalized to the incident flux. After a linear background subtraction, they were corrected for the active sample area, Lorentz and polarization factors [16]. The square root was taken to obtain the structure factor amplitudes. Out-of-plane measurements [17] were made as a function of the perpendicular momentum transfer along fractional order rods to determine the vertical displacements of the atoms participating in the reconstruction.

3. Results

The intensities of 276 peaks were measured at room temperature and, after considering the symmetry of the system, they reduced to 44 independent reflections, with an agreement factor of 0.103. Their square roots are proportional to the structure factor of the reflections, which depends on the geometrical arrangements of the atoms [18]

$$F_{h,k,l}=\sum_j f_j \exp\left[-2\pi_{i}(hx_j+ky_j+lz_j)\right] \times \exp\left(-\frac{B_jQ^2}{16\pi^2}\right), \qquad (3)$$

where f_j are the atomic scattering factors and B_j the isotropic Debye–Waller parameters, Q is the exchanged momentum, x_j, y_j and z_j are the atomic coordinates inside the unit cell, and (h,k,l) are the reflection Miller indices. The sum is over all the atoms j of the unit cell. To fit the experimental data we allowed atomic displacements with respect to the bulk positions and calculated the structure factors. The goodness of the fit is given by the χ^2 residual defined as

$$\chi^2=(N-p)^{-1} \times \sum_{h,k,l}\left(F_{\text{exp}}(h,k,l)-|F_{\text{calc}}(h,k,l)|\right)^2/\sigma^2(h,k,l), \qquad (4)$$

where N and p are the numbers of independent measured reflections and of the independent parameters used in the fitting, respectively. F_{exp} and F_{calc} are the observed and calculated structure factors, and σ is the statistical error of the measurement.

In Table 1 we report all the measured structure factors with their statistical error. We checked the stability of the sample by repeatedly measuring certain reference reflections. Because existing results [3,10,11,19,20] indicate that the Si(100)-(2×1) surface could be due to disordered and relaxed p(2×2) or c(4×2) reconstructions, we looked for fractional peaks related to these structures, but did not observe any intensity corresponding to them.

We tried to fit our experimental data assuming different models to minimize the χ^2 residual. We should point out that we only looked for solutions which induced minimal distortions in the Si–Si bulk bond distances. In our opinion, a fitting procedure performed without this constraint can lead to faulty solutions.

The first model we considered implied the presence of symmetric dimers. The best fit was achieved

Table 1
Measured structure factors F_{exp} of fractional order peaks and their standard deviations σ_{exp} as a function of h,k,l, which are in bulk reciprocal lattice units; the calculated factors F_{calc} have been obtained using the disordered model described in the text

h	k	l	F_{exp}	σ_{exp}	F_{calc}
1/2	0	0.20	59	7	54
1/2	0	0.50	49	6	56
1/2	0	0.75	38	5	45
1/2	0	1.00	36	4	38
1/2	0	1.25	37	5	38
1/2	0	1.50	40	5	32
1/2	1	0.20	40	5	35
1/2	1	0.50	44	5	37
1/2	1	0.75	48	6	38
1/2	1	1.00	33	4	32
1/2	1	1.25	26	3	27
1/2	1	1.50	29	4	25
1/2	2	0.20	31	4	30
1/2	2	0.50	36	4	32
1/2	2	0.75	32	4	26
1/2	2	1.00	17	4	23
1/2	2	1.25	19	4	24
1/2	2	1.50	16	4	21
1/2	3	0.20	17	3	17
1/2	3	0.50	21	3	18
3/2	0	0.20	71	9	72
3/2	0	0.50	91	11	84
3/2	0	0.75	61	7	63
3/2	0	1.00	47	6	43
3/2	0	1.25	40	5	44
3/2	0	1.50	37	5	39
3/2	1	0.20	41	5	44
3/2	1	0.50	47	6	51
3/2	1	0.75	38	5	49
3/2	1	1.00	40	5	35
3/2	1	1.25	43	5	43
3/2	1	1.50	63	8	57
3/2	2	0.20	44	5	49
3/2	2	0.50	63	8	60
5/2	0	0.20	32	4	29
5/2	0	0.50	44	5	41
5/2	0	0.75	19	3	21
5/2	0	1.00	8	5	8
5/2	0	1.25	8	5	20
5/2	0	1.50	18	4	13
5/2	1	0.20	9	2	10
5/2	1	0.50	26	3	23
7/2	0	0.20	20	3	19
7/2	0	0.50	17	3	19

having a lattice distortion from the bulk positions which propagates down to the eighth layer, similar to the structure proposed by Grey et al. [21] for the Ge(001)-(2 × 1) reconstruction. In this fitting we had a scale factor, six independent displacements and two Debye–Waller factors, one for the dimer atoms and the other for the remaining silicon atoms of the model, leading to nine independent parameters. The best χ^2 residual had a value of 2.1. The dimer bond length was 0.241 ± 0.003 nm, slightly longer than the bulk value of 0.235 nm and in excellent agreement with the value found by Jedrecy et al. [12] assuming the same model. All the other bond distances were practically equal to the bulk value.

To fit the experimental data using an ordered buckled-dimer model, recently proposed as the best solution for this system [22], we had to include several more free parameters with respect to the symmetric dimer model. In particular, we have to allow for asymmetric horizontal and vertical displacements of the silicon atoms of the first two layers. The best fit was achieved with a lattice distortion which propagates down to the eighth layer, similar to the symmetric dimer model. In this manner we were able to reduce slightly the square difference sum of Eq. (4), but because of the increase in the number of independent parameters p, the χ^2 residual was 2.4, higher than the symmetric model value. In this case the dimer bond length was 0.25 ± 0.01 nm, which is longer than the symmetric dimer value, much longer than the silicon bulk bond distance, and the result of Ref. [22]. We should point out that in our final structure, the differences between the bulk bond distances and the undistorted value are smaller than 2%. This is not verified for the model proposed in Ref. [22], where differences higher than 10% were reported.

A significant improvement of the fit quality was reached by assuming a disordered buckled dimer structure (statistical model), as first proposed by Rossmann et al. [13], again for the Ge(001)-(2 × 1) reconstructed surface. In their work, they showed that a dynamical model with anisotropic thermal parameters, and a statistical model where the positions of the atoms of the first two layers are split with occupancy factors of 0.5, are indistinguishable for their data. They had to assume displacements down to the tenth layer in order to fit their experimental data on the Ge(001)-(2 × 1) surface.

In Table 2 we list the coordinates in lattice units, and the associated displacements of all the atoms we have used in the model. In our case the best χ^2 residual was reached by splitting the position of the Si atoms of the first layer only, and by taking into account the following displacements: an independent x and an independent z displacement for each of the two atoms in the first layer (displacements: $d1$, $d2$, $d3$ and $d4$), one symmetric displacement along x for the second-layer atoms ($d5$), one vertical displacement for the silicon atoms of the third and fourth layers ($d6$), and two more symmetrical x displacements for the fifth and sixth layers ($d7$ and $d8$). In Fig. 3 we show a schematic view of the final structure, projected on the (x,z) plane, together with the atomic displacements used in the fit. We then have to consider the scale factor and the two Debye–Waller parameters, one for the atoms of the first two layers, and the second for the other atoms, obtaining 12 independent parameters. The best fit leads to a χ^2 residual of 1.34. In Table 1 we report the calculated structure factors for comparison with the experimental values, and in Fig. 2 we show the intensity variation along q_z of the most intense fractional-order peaks. In Table 3 we list the best fit values of the displacements. The Debye–Waller factor of the first two layers was 0.024 ± 0.007 nm^2, while for the inner layers it was 0.009 ± 0.007 nm^2. The dimer bond length of the final structure was 0.267 ± 0.007 nm with a dimer buckling angle of $20° \pm 3°$. The difference in height of the dimer silicon atoms is 0.092 ± 0.015 nm.

Table 2
Atomic positions with the associated displacements and occupancy factors of the model used for the best fit result; all the coordinates are in atomic cell unit ($a = 0.768$ nm, $b = 0.384$ nm, $c = 0.543$ nm)

Layer	x	y	z	Occ
1	$0.00+d1$	0.50	$1.75+d2$	0.5
1	$0.50-d3$	0.50	$1.75-d4$	0.5
1	$0.00+d3$	0.50	$1.75-d4$	0.5
1	$0.50-d1$	0.50	$1.75+d2$	0.5
2	$0.00+d5$	0.00	1.50	1
2	$0.50-d5$	0.00	1.50	1
3	0.25	0.00	$1.25-d6$	1
3	0.75	0.00	$1.25+d6$	1
4	0.25	0.50	$1.00-d6$	1
4	0.75	0.50	$1.00+d6$	1
5	$0.00-d7$	0.50	0.75	1
5	$0.50+d7$	0.50	0.75	1
6	$0.00-d8$	0.00	0.50	1
6	$0.50+d8$	0.00	0.50	1
7	0.25	0.00	0.25	1
7	0.75	0.00	0.25	1

In the literature very few experimental determinations of the dimer geometry exist which can be used for comparison with our result. The dimer projection on the surface plane has been determined either by surface X-ray diffraction [12] and by low-energy ion scattering [23], finding a value of 0.24 ± 0.01 nm, while for the dimer bond length a value of 0.254 ± 0.015 nm was obtained by low-energy electron diffraction data analysis [24]. Moreover, recent results of X-ray standing wave measurements of Ge on Si(001) [25] have shown that germanium atoms form asymmetric dimers with a bond length of 0.260 ± 0.004 nm and a buckling angle of $12.1 \pm 0.2°$ and X-ray diffraction experiments on the low-temperature clean Ge c(4 × 2) reconstruction [26] indicate the presence of buckled dimers with an angle of $19 \pm 1°$ and a bond length 4% longer than the bulk value. All these values agree, within experimental errors, with our result, and indicate that discrepancies still exist with most of the theoretical calculations predicting a dimer bond length close to or shorter than the bulk Si–Si bond value [4,5,8].

In our proposed model the second-layer atoms have displacements of the same value but opposite directions along the x-axis, moving inwards with respect to the dimer. These displacements cause a rotation of the hexagonal structure, pushing down the 3a and 4a silicon atoms, pulling up the 3b and 4b silicon atoms, and inducing an outward displacement with respect to the dimer of the fifth- and sixth-layer atoms. We assumed that all the displacements of the atoms of the third and fourth layer have the same magnitude because we do not have enough resolution to distinguish between them.

Considering the two possible orientations of the buckled dimer, it seems that the bonding distances of these two atoms with respect to the second-layer atoms are either very long (0.259 nm) or very short (0.220 nm). This should induce large displace-

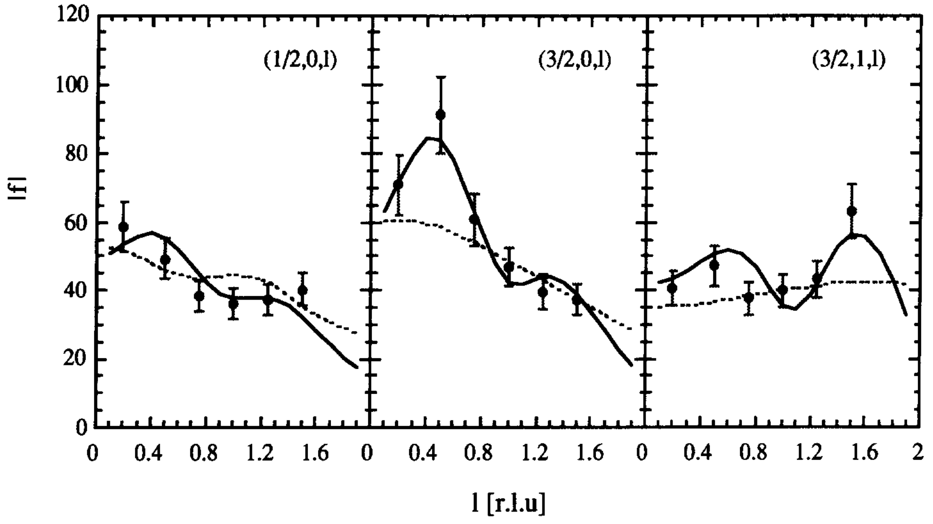

Fig. 2. Experimental structure factors for the most intense measured rods. The lines have been calculated using the model described in the text. The dashed lines have been calculated using the atomic cohordinates predicted by theory [28].

Table 3
Displacement values of the best-fit result, which led to a χ^2 residual of 1.34; the quoted errors are determined by the fitting procedure and do not include any systemic error

	Displacement	
Number	Value in lu	Value in nm
*d*1	0.065 ± 0.006	0.050 ± 0.005
*d*2	0.057 ± 0.018	0.031 ± 0.010
*d*3	0.108 ± 0.004	0.083 ± 0.002
*d*4	0.113 ± 0.021	0.061 ± 0.011
*d*5	0.009 ± 0.001	0.0069 ± 0.0008
*d*6	0.005 ± 0.004	0.0027 ± 0.0022
*d*7	0.007 ± 0.001	0.0054 ± 0.0008
*d*8	0.004 ± 0.001	0.0031 ± 0.0008

ments from the original positions of the second-layer atoms, because the bond's chemical nature is similar to the bulk, and the distance cannot be too different from the bulk case. We also explored the possibility that the second-layer atoms move freely in the *x*,*z* plane, maintaining a double site with 50% occupancy, as for the dimer atoms. However, the fitting shows that the second-layer atoms: (i) do not split in position in the *x*,*z* plane as in the disordered model proposed by Rossman et al. [13], (ii) have a *z* displacement equal to zero, and (iii) have small *x* displacements equal in magnitude and with opposite directions, causing them to move inward to the dimer symmetrically. Different displacements along the *z* direction or along the *x* direction for the two atoms would indicate that the disordered structure might be an evolution from an ordered (2 × 1) buckled dimer structure. The most likely possibility is that these atoms move along *y*, as happens in the c(4 × 2) structure [27], but our experiment was not sensitive to these displacements because they break the (2 × 1) symmetry, and we only collected peaks corresponding to the (2 × 1) reconstruction. To determine these displacements, we need to measure the intensity of peaks corresponding to the c(4 × 2) or to the p(2 × 2) reconstructions, but we could not observe any of these at room temperature emerging from the background.

Our results indicate the presence of disordered buckled dimers, and are consistent with a reconstruction of higher order than (2 × 1). Our final structure is thus compatible with a move from either a p(2 × 2) or a c(4 × 2) structure towards one in which the buckling directions of the dimer are uncorrelated. This is congruous with reported results [3] of scanning tunneling microscopy measurements, where zones with (4 × 2) and (2 × 2) reconstructions were observed at low temperature, while at room temperature dimers rapidly switch orientation leading to an averaged symmetric (2 × 1) structure, and results of core level spectroscopy studies [10], which show the close similarity between the spectra measured at low temperature for the c(4 × 2) reconstruction and at room temperature for the (2 × 1) reconstruction.

Recent theoretical results [28] show that the p(2 × 2) and c(4 × 2) structures have much lower energy than the (2 × 1) reconstruction. This is in agreement with our best fit structure, which is likely to be a disordered version of a c(4 × 2) or of a p(2 × 2) reconstruction. We have to compare our result with the theoretical calculations regarding these higher-order reconstructions, which predict a dimer buckling Δz of 0.077 nm [26] (to be compared with our 0.092 ± 0.015 nm) and a buckling angle of 17.5° [29] (ours is 20° ± 3°). Nevertheless, the predicted dimer bond length is of the order of the Si–Si bulk distances, and much shorter than our value.

A further comparison with respect to theoretical calculation, carried out using the Carr–Parrinello method [30], shows a good general agreement. The theoretical results indicate that the (2 × 1) structure does not exist even at room temperature, and that a p(2 × 2) or a c(4 × 2) reconstruction is preferred. The dimer is tilted with respect to the crystal plane by an angle of 18.4° or 16.9° and a buckling of 0.068 or 0.062 nm for the two reconstructions, respectively, in agreement with our best fit values. The dimer bond length is 0.238 nm shorter than ours and other experimental results. A very good agreement is, however, shown by the displacements of the other inner layers [31]. In fact, the second-layer atoms have the same z coordinates, show a symmetric movement to the dimer of about 0.011 lu with respect to our experimental value of 0.009 ± 0.001, and a symmetric y displacement which we cannot determine with our data set. The third and fourth layers show the same type of vertical displacements as our model, even if their absolute values are not the same for all the atoms and slightly larger than our values (theory 0.009 nm, our value 0.0027 ± 0.0022 nm). In Fig. 3 we also show the rods calculated using the atomic coordinates obtained by theoretical results [31]. In this case the reduced χ^2 has a value of 5.1. We also tried to fit our data assuming the dimer geometry predicted by the theory, letting the atoms of the deeper layers be free to move, but the best reduced χ^2 we found was 2.5, a value significantly worse than our best fit. We can therefore conclude that there is an overall agreement between the predicted and measured surface symmetry of the Si(2 × 1) reconstruction. However, the measured dimer bond length is longer than the theoretical value.

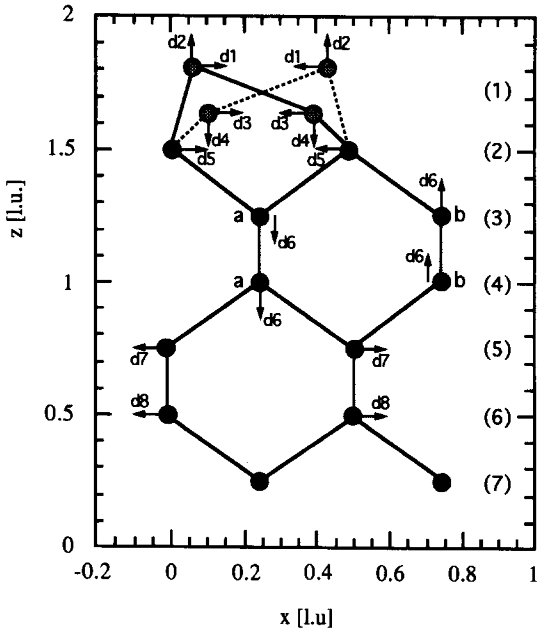

Fig. 3. Structure of the Si(001)-(2 × 1) reconstruction projected in the x,z plane. The atoms of the dimer (dashed points) have been split in two sites with an occupancy factor of 0.5 according to the statistical model. The arrows show the displacements and their constraints used in the best fitting procedure.

4. Conclusions

We studied the room-temperature (2 × 1) reconstruction of the clean Si(001) surface by measuring the X-ray diffraction from fractional-order peaks. Our data have been discussed in terms of symmetric and asymmetric dimer models. Our best fit is consistent with the presence of disordered asymmetric dimers which induce atomic relaxations down to the sixth layer. Because the second-layer atoms only show a symmetric displacement inward to the dimer, we conclude that the observed (2 × 1) structure is a disordered higher-order reconstruction, either p(2 × 2) or c(4 × 2). This is in agreement with most of the experimental data and with the most recent theoretical results, which indicate that the (2 × 1) reconstruction is not stable even at room temperature. Our best-fit dimer geometry has a bond length of 0.267 ± 0.007 nm with a buckling angle of $20 \pm 3°$. These values agree, within experimental errors, with the experimental determinations existing in the literature and, in the case of the buckling angle only, with the values predicted by theoretical calculations. However, a strong discrepancy exists between our best-fit dimer bond length and the theoretical values, which are very similar to the bulk Si–Si bond distance. For a better understanding, we advise low-temperature X-ray diffraction studies of the clean Si(001) surface to determine the structure of the most stable c(4 × 2) reconstruction. In this manner the dimer bond length would be measured exactly without suffering from distortions due to the disordered geometry. Moreover, temperature-dependent studies of anharmonic effects on the Debye–Waller parameters would also confirm that the observed room-temperature (2 × 1) reconstruction is a disordered version of a higher-order structure.

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