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Hydrogen induced missing row reconstruction of Fe(211)

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Abstract

We present quantitative structure determinations by low energy electron diffraction of both the clean Fe(211) phase and a drastic (1×2) reconstruction induced by hydrogen under thermal activation. For the clean surface we find a registry shift between the first two atomic layers and an oscillatory multilayer relaxation in agreement with earlier work. The reconstructed (1×2) phase is shown to be of the missing row type, whereby every second close packed atomic row is removed. The Pendry R -factors, $R = 0.16$ and 0.19 for the clean and reconstructed surface respectively, are convincingly low. Additionally, the missing row reconstruction accounts quantitatively for the observed brightness of extra diffraction spots. The removal of atomic rows entails considerable movements of second and third layer iron atoms, i.e. pairing and buckling.

1. Introduction

Due to its chemical activity hydrogen is well known to affect the structure of a substrate by adsorption (for a review see Ref. [1]). In most cases the reconstruction of the substrate is of the displacive type, whereby the displacements of atoms can vary from only a few hundredth of an Ångström as e.g. for H/Rh(110) [2], H/Fe(110) or H/Ni(111) [3] to a few tenths of an Ångström as for e.g. the row pairing reconstruction of H/Ni(110) and H/Pd(110) [4]. In contrast, bond breaking reconstruction induced by hydrogen seems to be rare. The only cases we know of are the ‘streaked’ (1×2) phases of hydrogen on Ni(110) and Pd(110) which develop under thermal activation at temperatures $T > 200$ K

leading to a missing row reconstruction as argued in Ref. [4] and shown for H/Ni(110) by scanning tunnelling microscopy in Ref. [5]. Every second close packed atomic row in $[\bar{1}10]$ direction is removed and added somewhere on the surface again with (1×2) periodicity (combined missing and added row model). However, to our knowledge no quantitative structure determination is available for such a hydrogen induced missing row reconstruction of close packed atomic rows.

In the following we report on a hydrogen induced (1×2) missing row reconstruction of the Fe(211) surface. The general aspects of the hydrogen adsorption on Fe(211) are described in detail elsewhere [6,7]. So, in the present paper we mainly focus on the structure determination of the reconstructed phase performed by quantitative low energy electron diffraction (LEED). In the next section experimental details are given whilst Section 3 describes the basics of the LEED intensity calculation. Section 4

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presents the structure determination of the clean surface which confirms earlier work [8]. This is followed by the determination of the hydrogen induced (1×2) missing row reconstruction and Section 6 concludes the paper.

2. Experimental

The experiments were performed in a standard stainless steel UHV apparatus (base pressure 5×10^{-11} mbar) provided with a four grid back view LEED optics which was also used as a retarding field analyser for Auger measurements. Additionally, a quadrupole mass spectrometer for thermal desorption spectrometry and a Kelvin probe for work function measurements were available. Cryogenic temperatures ($T \geq 35$ K) could be reached through a special sample holder contacted to a closed cycle helium gas refrigerator as described in detail elsewhere [9]. The sample was mechanically polished to within 0.5° of the (211) orientation. Its purity was 99.99% with S, C and P as main impurities. The sample was precleaned by a procedure carried out in the Max Planck-Institut für Eisenforschung (Düsseldorf): Annealing in H_2 (1 bar, 970–1120 K, several weeks) produced a sample with sulphur largely removed. In situ preparation by sequences of neon-ion bombardment (2–3 μA , 500 V, 670–920 K, 20 min–several hours) followed by thermal annealing (920 K) was successful to produce a practically clean surface which after a final flash exhibited a bright, sharp and low background (1×1) LEED pattern. Residual gas adsorption, in particular CO, was found to influence the hydrogen adsorption phases considerably. So, each exposure of the sample to hydrogen ($\geq 10^{-9}$ mbar) was preceded by a flash to 930 K to make CO desorb.

Whilst a number of commensurate superstructures ($c(2 \times 6)$ –8H, $(2 \times 1)_{\text{plg1}}$ –2H, $c(2 \times 6)$ –16H, $c(2 \times 4)$ –12H, (1×3) –5H and (1×1) –2H) with low extra spot intensities develops with hydrogen adsorption at low temperatures a (1×2) phase with very bright superstructure spots forms when the system is annealed at above 200 K [6,7]. The brightness of the beams indicates the existence of a drastic reconstruction whereby possibly bond breaking between substrate atoms is involved. The necessary hydrogen

coverage for the reconstruction is not critical, we observed the (1×2) phase for coverages between 0.2 and 1.2 monolayers. (In order to express that the (1×2) superstructure is formed mainly by substrate reconstruction we will call it $(1 \times 2)_{\text{rec}}$ in the following.) However, without thermal activation the $(1 \times 2)_{\text{rec}}$ is not observed. This indicates that some mass transport may be connected with the formation of this phase. Usually the superstructure spots are streaked similar to the reconstructed phases of H/Ni(110) and H/Pd(110) [4,5]. However, by careful preparation the streaks can be made to disappear leaving round spots [7].

Quantitative LEED intensity measurements were carried out using a computer controlled video technique. As described in detail elsewhere [10,11] a video camera views the diffraction pattern from outside the UHV equipment and the video signal is evaluated on-line by a computer. This allows high speed measurements of $I(E)$ spectra with a maximum rate of one intensity data point per energy and beam within the time of a video half frame, i.e. 20 ms (European norm). This speed is essential to limit the influence of residual gas adsorption.

Intensity data were measured at about 40 K with the primary electron beam normal to the surface for both the clean surface and the $(1 \times 2)_{\text{rec}}$ phase. However, for bcc (211) surfaces with only one symmetry plane (along the $[1\bar{1}\bar{1}]$ direction), normal incidence is difficult to control with high accuracy. So, only in-symmetry plane incidence could be adjusted as usual, namely by comparison of symmetrically equivalent beams (e.g. the 01 and $0\bar{1}$ beams). For the comparison the Pendry R -factor [12] was used and symmetric incidence was believed to be of sufficient accuracy when $R < 0.05$ between spectra of equivalent beams. Normal incidence within the symmetry plane was adjusted by eye only. A possible misalignment was left to be considered in the course of the structure determination of the clean surface whereby the angle of misalignment was treated as an additional fitting parameter. Intensity spectra of 9 symmetrically non equivalent beams (up to the 3rd order) were measured for the clean surface. The maximum energy was 500 eV corresponding to a total energy width of $\Delta E = 3515$ eV as summed over all beams. For the hydrogen covered phase the maximum energy was 250 eV in order to limit the

necessary computational efforts for the intensity calculations. In addition to the 9 integer order spots 6 half order spots were measured (up to the order $0\frac{5}{2}$) resulting in a data base of total energy width $\Delta E = 2260$ eV. The energy averaged intensity level $\langle I_h \rangle$ of half order spot intensities compared to $\langle I_s \rangle$ of substrate spots is $r = \langle I_h \rangle / \langle I_s \rangle \approx 39\%$. This indicates the presence of a substantial substrate reconstruction.

3. Intensity calculations

The full dynamical intensity calculations for the clean surface were carried out using standard computer programs [13,14]. A total of 10 phase shifts ($l_{\max} = 9$) relativistically calculated and spin averaged for bcc iron proved to be sufficient to describe the electron scattering by iron atoms up to 500 eV. They were corrected for thermal diffuse scattering [13,14] using the bulk Debye temperature $\Theta_b = 420$ K for bulk iron atoms and an adjustable surface Debye temperature Θ_s for top layer atoms. Layer diffraction matrices were calculated by matrix inversion and layers were stacked by the layer doubling scheme. The electron attenuation was described by an energy independent imaginary part V_{oi} of the inner potential which was fitted as a non structural parameter. The real part of the inner potential was adjusted in the course of the theory-experiment fitted as usual.

In view of the strong superstructure spot intensities scattering from hydrogen was neglected for the analysis of the $(1 \times 2)_{\text{rec}}$ phase in a first step. This seems to be reasonable because of the low scattering strength of hydrogen compared to iron. It is illustrated in Fig. 1 which displays the energy dependent ratio of the total cross sections of the two atoms. Above 100 eV the ratio is smaller than 3% which in view of the 39% intensity level of superstructure spots compared to substrate spots is negligible. For the test of different first substrate layer reconstruction models accounting for the (1×2) superstructure pattern the above described conventional methods were used. With the most promising model found a structural refinement procedure for the determination of a possible reconstruction of deeper layers was started in a second step using the perturbative tensor

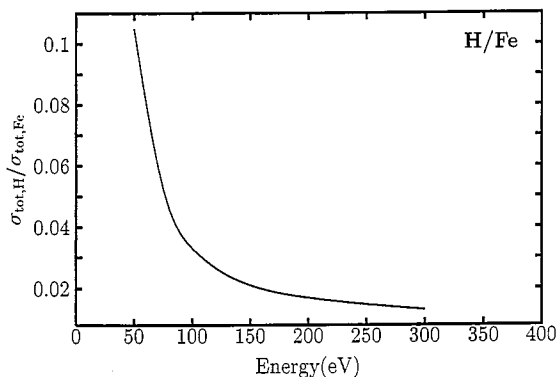


Fig. 1. Ratio $\sigma(H)/\sigma(Fe)$ of total elastic electron scattering cross sections of hydrogen and iron as function of energy (maximum angular momentum considered: $l_{\max} = 9$).

LEED method [15–17]. The starting structure was used as the reference. In a third step both conventional methods and tensor LEED were tried to determine the hydrogen position on the reconstructed substrate. Theoretical and experimental data were compared by means of the Pendry R -factor [12]. For both the clean and hydrogen covered surface the parameter space was scanned in reasonable areas, i.e. no structural search procedure was used to avoid landing in a local rather than a global R -factor minimum. Error limits for the structural parameters determined were estimated by the variance of the Pendry R -factor $\text{var}(R) = R_{\min} \sqrt{8V_{oi}/\Delta E}$ [12].

4. Structure analysis of the clean surface

As mentioned in the introductory part the clean Fe(211) surface was already successfully analyzed earlier by Sokolov et al. [8] who found an oscillatory multilayer relaxation as usual for clean metal surfaces. Additionally, however, a registry shift between the first and second layer and the second and third layer was detected (a hard sphere model of the surface is displayed in Fig. 2). Though the error limits given were rough estimates only, the Fe(211) surface seems to be one of the rare cases where such a registry shift has been detected. As our data base $\Delta E = 3515$ eV is fairly broad there is the chance to determine the registry shift with high reliability.

The strategy of the intensity analysis is as follows. In a first step only geometrical parameters, i.e.

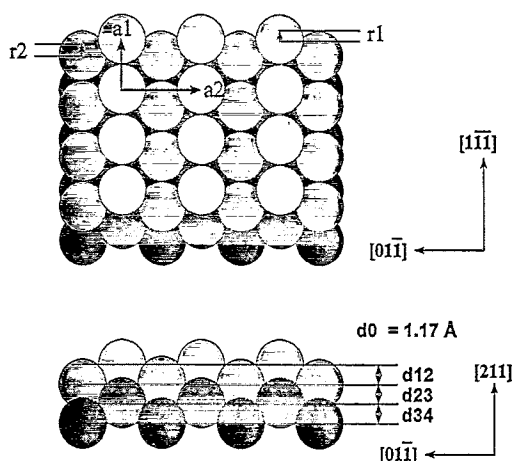


Fig. 2. Hard sphere model of the clean Fe(211) surface in top and side view.

interlayer distances $d_{i,i+1}$ ($i = 1, 2, 3$) and registry shifts r_i ($i = 1, 2$) were varied for normal primary beam incidence. Then with the best fit geometry fixed, the angle of incidence within the symmetry

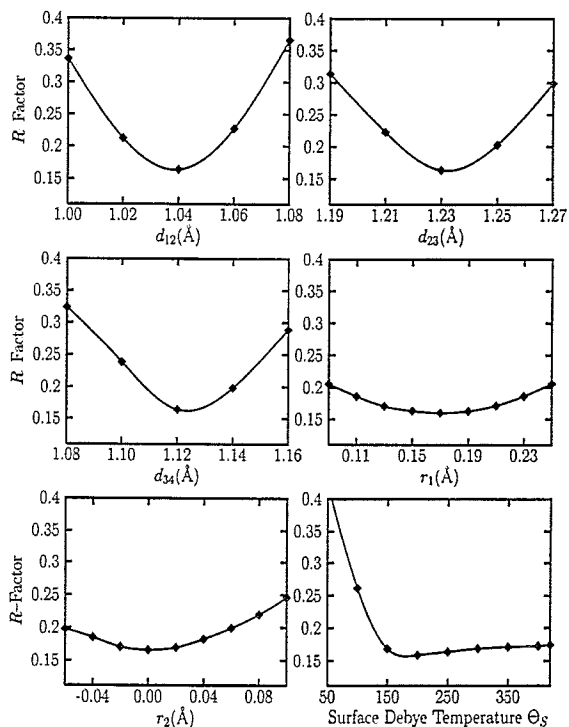


Fig. 3. Variation of the Pendry R -factor as a function of the geometrical parameters and the surface Debye temperature of the clean Fe(211) surface.

Table 1

Comparison of interlayer distances and registry shifts found by Sokolov et al. [8] with those determined in this work for the clean Fe(211) surface (the bulk layer distance is $d_0 = 1.17 \text{ \AA}$). All registry shifts are given with respect to bulk layer coordinates.

	Sokolov et al. [8]	this work
d_{12} (Å)	1.05 ± 0.03 ($-10\% \pm 3\%$)	1.04 ± 0.01 ($-11 \pm 1\%$)
d_{23} (Å)	1.23 ± 0.03 ($+5\% \pm 3\%$)	1.23 ± 0.01 ($+5 \pm 1\%$)
d_{34} (Å)	1.15 ± 0.04 ($-2\% \pm 3\%$)	1.12 ± 0.01 ($-4 \pm 1\%$)
r_1 (Å)	$+0.24 \pm 0.03$	$+0.17 \pm 0.04$
r_2 (Å)	-0.037 ± 0.03	$\pm 0.00 \pm 0.04$

plane was varied as well as the non structural parameters such as the surface Debye temperature and imaginary part of the inner potential. Subsequently, for the best fit values of these parameters the geometrical parameters were readjusted. A clear minimum of the R -factor, $R = 0.16$, was found. The angle of incidence, the surface Debye temperature and the imaginary part of the inner potential are optimized at $\vartheta = 1^\circ$, $\Theta_s = 200 \text{ K}$ and $V_{oi} = 5.0 \text{ eV}$, respectively. The variation of the R -factor as a function of the geometrical parameters and of the surface Debye temperature is displayed in Fig. 3. The geometry found is compared with the structural values reported by Sokolov et al. in Table 1. A selection of experimental and best fit spectra are compared in Fig. 4.

Obviously, within the limits of error our results compare very well to those of Sokolov et al. However, we find no indication for a registry shift of the second layer ($r_2 = 0$). Also, the value found for the shift of the first layer, $r_1 = 0.17 \text{ \AA}$, is smaller than their value but is definitely outside the limits of error. The shift brings the surface atoms nearer to 3-fold coordination with second layer atoms, though ideal 3-fold coordination would be reached only with r_1 as large as 0.4 \AA .

5. Structure analysis of the hydrogen induced $(1 \times 2)_{\text{rec}}$ phase

As mentioned in Section 2 the half order spots of the $(1 \times 2)_{\text{rec}}$ phase are very bright (39% of substrate intensities on energy average) and thus cannot be due to hydrogen scattering alone. A substantial re-

construction induced by hydrogen adsorption at temperatures above about 200 K must have taken place. In order to determine the new substrate structure scattering from hydrogen can be neglected.

Of course a number of atomic arrangements can account for the observed (1×2) symmetry. For the (110) surfaces Pd and Ni a hydrogen induced pairing of linearly close packed atomic rows was found leading to a (1×2) reconstruction of the substrate (e.g. Ref. [4]). As the bcc (211) surface exhibits also such close packed rows a “row pairing” reconstruction should certainly be checked. On the other hand it is well known that adsorbates can also induce much more serious reconstructions whereby not only local displacements (as in the pairing row reconstruction) but complete removal of surface atoms is involved. So, e.g. alkali atoms adsorbed on Cu (110) [18,19] or Pd (110) [20] remove every second atomic row leading to a “missing row” structure. As such a dramatic reconstruction was also reported to be induced by hydrogen on Ni (110) and Pd (110) [4,5] it must be checked for as well. Also non close packed atomic rows can be removed leading to a (2×1)

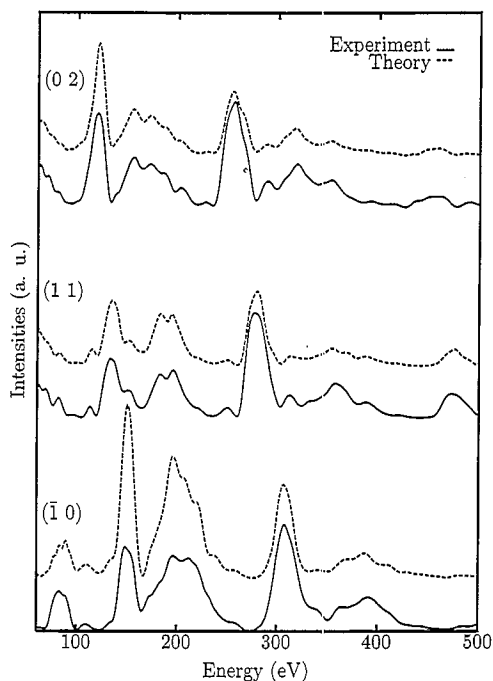


Fig. 4. Comparison of experimental and best fit spectra of clean Fe (211) for an off-normal incidence of $\vartheta = 1^\circ$ within the surface symmetry plane.

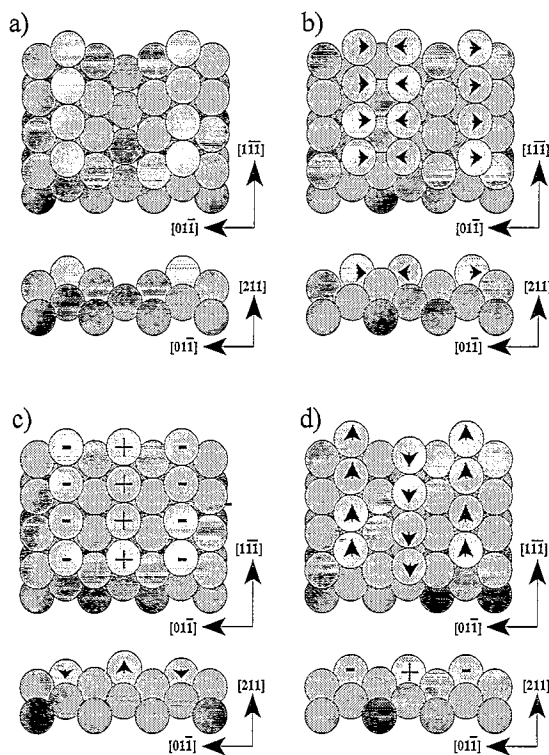


Fig. 5. Different reconstructions of the top Fe layer: (a) missing row, (b) pairing row, (c) buckling row, and (d) zig-zag-reconstruction.

missing row superstructure as known for e.g. O/Cu (110) [21–25] and, interestingly, O/Fe (211) [26].

Therefore, we checked in a first step for possible types of first layer reconstructions neglecting any reconstructions of subsurface layers. Figs. 5a and 5b display the missing and pairing row models. Additionally, we checked for a buckled row reconstruction in which every second row is pulled out of or pushed into the surface by a certain amount (Fig. 5c), and for a zig-zag reconstruction in which atomic rows are displaced along their linear direction with alternating sign (Fig. 5d). Fortunately, all models except the missing row model can be clearly ruled out. Its R -factor with interlayer distances fitted but subsurface layers left unreconstructed is $R = 0.48$ while the other models yield values not better than 0.61. If registry shifts are taken into account the R -factor of the missing row model improves from 0.48 to 0.36 while the best of the other models yielded only $R = 0.56$. Even more important and

convincing, however, is the fact that only the missing row model accounts for the experimentally observed high super-structure spot intensities, while the other models yield only weakly reconstructed best fit geometries with superstructure spot intensities small compared to experiment.

Of course the R -factor level achieved so far for the missing row model leaves much room for improvement of the fit. There are many free parameters to be adjusted if one allows for the reconstruction also of deeper layers. Such reconstructions are well known to exist in other cases of top layer missing row structures. There can be row pairing in the second layer and buckling in the third layer which, in addition may exhibit some zig-zag reconstruction along their linear direction as well. Moreover, the situation is complicated by the registry shift which may have survived the reconstruction with a certain change and now may even exist in deeper layers.

All the possible displacements considered are indicated in Fig. 6. They are consistent with the experimentally observed mirror plane. There is a total of 10 geometrical parameters to be adjusted. As the atomic movements can be expected to be small compared to the atomic diameter this is an almost ideal case for tensor LEED. Therefore, we took the geometry of the best fit achieved so far as a reference structure with non-structural parameters taken

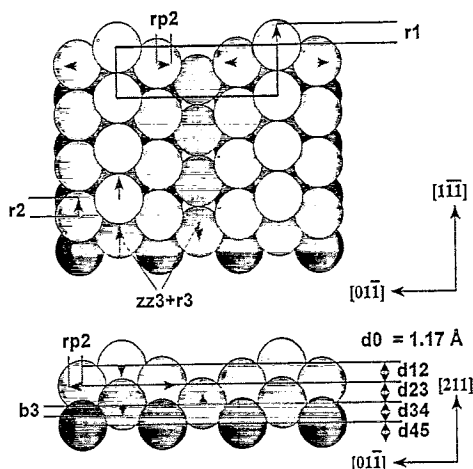


Fig. 6. Model of the missing row reconstruction with possible displacements of subsurface atoms (r_3 describes a registry shift of the 3rd layer, zz_3 allows for an additional zig-zag reconstruction in that layer).

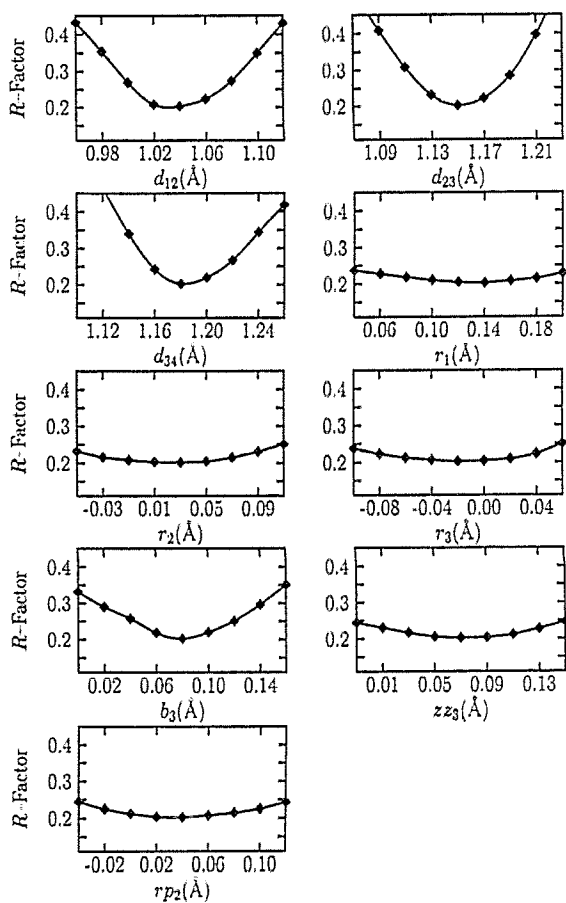


Fig. 7. Variation of the Pendry R -factor as a function of the geometrical parameters of the hydrogen induced $(1 \times 2)_{\text{rec}}$ missing row reconstruction of Fe(211).

from the results for the clean surface and simulated the displacements of atoms off these reference positions by tensor LEED. A clear minimum was found corresponding to a Pendry R -factor $R = 0.19$ which is convincingly low for a structure of that complexity (the same value holds for both the integer and half order spots). Fig. 7 displays the behaviour of the Pendry R -factor for various parameters in the vicinity of the global best fit. Apparently, among all parameters the buckling in the third substrate layer influences the spectra most and amounts to $2 \times 0.08 \text{ \AA} = 0.16 \text{ \AA}$ whereby simultaneously a zig-zag reconstruction is involved. There is a substantial second layer row pairing with a shift of 0.04 \AA for each atomic row which, however, is within the limits of error. The same holds for the registry shifts of the

second and the third layer. The registry shift between the first layer has survived indeed, though with a slightly reduced amplitude of 0.14 Å with respect to the bulk layer coordinates. Since there is an additional registry shift found for the second layer, a relative shift between the first two layers of only 0.11 Å results compared to the 0.17 Å for the clean surface. Table 2 puts all best fit structural parameters together including their error limits as again derived from the variance of the R -factor with $\Delta E = 2260$ eV. Fig. 8 compares a selection of experimental and calculated best fit spectra.

In addition to yielding a convincing minimum R -factor the best fit model should also produce the experimentally observed ratio between average intensities of fractional and integer order spots, $r_{\text{exp}} = 39\%$. The calculated value turns out to be $r_{\text{cal}} = 47\%$, i.e. higher than the experimental value. However, in view of the fact that theory assumes a perfect surface with long range order reconstruction everywhere, i.e. neglects disorder and surface roughness always present on a real surface, the calculated value should even be higher than the experimental value. So, $r_{\text{cal}} = 47\%$ versus $r_{\text{exp}} = 39\%$ can be interpreted to support our best fit model in addition to the good R -factor agreement.

In a final effort we tried to fix the adsorption position of hydrogen whereby only 3-fold coordinated high symmetry sites were tried which are frequently occupied by hydrogen [1]. In a first step we have tested all reasonable adsorption models

Table 2

Best fit structural parameters as defined in Fig. 6 for the hydrogen induced $(1 \times 2)_{\text{rec}}$ reconstruction of Fe(211). All registry shifts are given with respect to bulk layer coordinates.

parameter	best fit	error
d_{12} (Å)	1.04 (−11%)	±0.03
d_{23} (Å)	1.15 (−2%)	±0.02
d_{34} (Å)	1.18 (+1%)	±0.02
d_{45} (Å)	1.17 (+0%)	±0.02
r_1 (Å)	+0.14	±0.06
r_2 (Å)	+0.03	±0.06
r_3 (Å)	−0.02	±0.06
b_3 (Å)	±0.08	±0.03
zz_3 (Å)	±0.07	±0.06
rp_2 (Å)	±0.04	±0.06

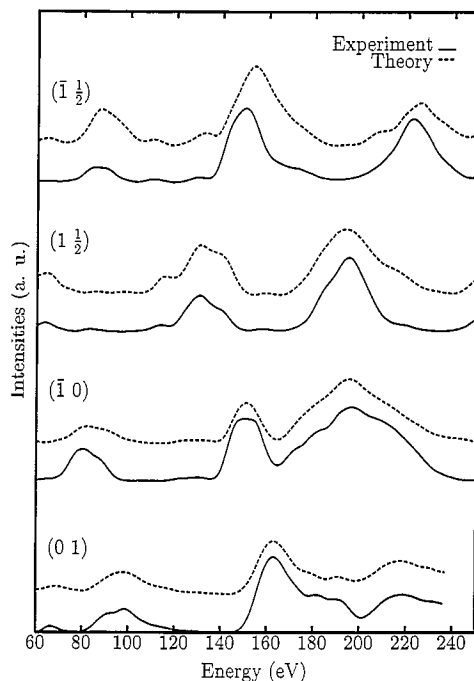


Fig. 8. Comparison of experimental and calculated best fit spectra for the hydrogen induced $(1 \times 2)_{\text{rec}}$ reconstruction of Fe(211) with hydrogen scattering neglected.

corresponding to a hydrogen coverage of $\Theta_{\text{H}} = 1$ with the substrate reconstruction fixed at the best fit configuration. For the most promising model a full variation of all parameters, i.e. hydrogen position and substrate reconstruction has been performed by tensor LEED. Unfortunately, however, we could not improve the R -factor level with any adsorption configuration. This is because the additional scattering of hydrogen, i.e. its contribution to both fractional and integer order spots is extremely weak compared to the intensity level produced by the clean missing row reconstructed substrate. In the present case we could not decide whether a small detail in an intensity spectrum is caused by additional hydrogen scattering or by some modification of the substrate geometry. The situation is different from that of e.g. (1×1) -2H/Rh(110) where hydrogen also fails to produce extra spots [27]: With an unreconstructed substrate there are only a few parameters to be readjusted and so the information about the adsorption geometry is detectable. In the present case the substrate geometry is so complex that any weak adatom scattering seems easy to be simulated by a small modification of some substrate parameters.

6. Conclusion

The analysis of the clean surface confirms and determines with high accuracy the presence of a registry shift between the first two layers of Fe(211) in addition to the oscillatory multilayer relaxation usually observed for non close packed metal surfaces. Hydrogen adsorption in a wide range of coverage ($0.2 < \Theta < 1.2$) induces a massive substrate reconstruction when sufficient thermal activation is provided ($T > 200$ K). The reconstruction proves to be of the missing row type and so is fully consistent with the high temperatures necessary to produce the structure by mass transport, i.e. removal of atomic rows at one area of the surface and adding them at some other place in the same (1×2) symmetry. Though a similar reconstruction has also been reported for H/Ni(110) [4,5] the present work to our knowledge is the first quantitative structure determination of a hydrogen induced removal of linearly close packed rows. Interestingly, oxygen adsorption also removes atomic rows from the surface [26] but these rows are not close packed and directed along $[0\bar{2}2]$, i.e. orthogonal to $[1\bar{1}\bar{1}]$ leading to a (2×1) superstructure. As usual, the (1×2) missing row reconstruction is not without consequences with respect to the structure of deeper layers. There is considerable pairing of rows and buckling of layers. The registry shift determined for the clean surface survives the reconstruction process though with slightly reduced amplitude. Also, it seems to spread to deeper layers. The reconstruction found not only reproduces the experimental intensity spectra (Pendry R -factor $R = 0.19$) but also the high average intensity level of superstructure beams. Unfortunately, this high level in connection with the complexity of the reconstruction prohibits the determination of the hydrogen adsorption site because it turns out that hydrogen scattering is too weak to be discriminated from small changes in the substrate geometry.

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