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Multilayer relaxation of body-centred-cubic Fe{211}

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Abstract. The atomic structure of the clean surface of BCC Fe{211} was analysed by low-energy electron diffraction (LEED). Thirty intensity–energy spectra (19 non-equivalent) for three directions of incidence were collected and compared with calculations by means of a reliability factor. The surface structure consists of a first-layer registry shift of 0.24 ± 0.03 Å with respect to the second layer, a second-layer registry shift of 0.037 ± 0.03 Å with respect to the third layer in the direction opposite to the first-layer registry shift, a first interlayer spacing d_{12} = 1.05 ± 0.03 Å (bulk value is 1.17 Å), a second interlayer spacing d_{23} = 1.23 ± 0.03 Å and a third interlayer spacing d_{34} = 1.15 ± 0.04 Å. The first-layer registry shift is along a ⟨111⟩ direction such as to decrease the difference between nearest and next-nearest neighbour bond lengths among atoms in the top two layers. The overall agreement between theory and experiment as measured by the reliability factor of Zanazzi and Jona is 0.111.

1. Introduction

In recent years there has been a fruitful interaction of theory and experiment on the subject of surface relaxation of metal crystals. Early calculations based on empirical two-body potentials fitted to various bulk properties (Burton and Jura 1967, Bonneton and Drechsler 1970, Wynblatt and Gjostein 1970) predicted *outward* relaxation of the top metal layers. However, experimental LEED (low-energy electron diffraction) results on Al{110} (Jepsen *et al* 1972, Laramore and Duke 1972, Martin and Somorjai 1973) indicated a substantial *contraction* of the first interlayer spacing. Finnis and Heine (1974) proposed a simple model for the 'smoothing' of the electronic charge density at the surface with the resulting electrostatic force on the top layer ions driving an inward relaxation. This model also predicted that the more densely packed surfaces Al{100} and A{111} would exhibit substantially less contraction than Al{110}, in qualitative agreement with the experiments of Martin and Somorjai (1973). In the next few years increasingly accurate results for a variety of metal surfaces appeared (for a review see Jona 1978), indicating that most cases exhibit a contraction of the first interlayer spacing (d_{12}) of 0–15%. Further theoretical work by Ma *et al* (1978) included both empirical

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interatomic potentials and the effect of electronic density smoothing, and when applied to the Cu{001} and Fe{001} surfaces gave reasonable quantitative agreement with experiment. An interesting feature of the work of Ma *et al* was the prediction of a multilayer oscillatory relaxation of interlayer spacings, a feature which had also appeared in some of the earlier (and inaccurate) studies using bulk-like pair potentials (for example, Jackson 1971). However, for the cases of Cu{001} and Fe{001} the predicted relaxations of d_{23} and d_{34} (interlayer spacings between second and third, and third and fourth layers, respectively) were too small to be accessible by present experimental methods. More recently, Landman *et al* (1980) used a simple electrostatic scheme and for three models of the electronic density calculated the multilayer relaxation of the low-index faces of Al, Li, Na and Cu. In particular, results for the open faces BCC{111} and FCC{110} (BCC = body-centred cubic, FCC = face-centred cubic) predicted damped oscillatory relaxations of the interlayer spacings large enough to be detected experimentally. Experiments on Cu{110} (Davis *et al* 1979, Adams *et al* 1982) and Al{110} (Nielsen *et al* 1982) confirmed the general picture but found smaller and more highly damped relaxations than predicted. Barnett *et al* (1983) have calculated the surface relaxation of Al{110} using a method based on the minimisation of the total energy of the semi-infinite crystal and which included a realistic calculation of the electronic response to variations of ion positions, and obtained good *quantitative* agreement with experiment.

The question arises as to whether multilayer oscillatory relaxations are a general feature of all metal surfaces. It is important to study new systems so as to determine possible trends. Theoretical predictions indicate that relaxations are largest for surfaces with relatively open faces such as BCC{111} and FCC{110}. Fe{211}, with a packing fraction of 0.481 is thus expected to be a good candidate for study of multilayer relaxation. In addition, the low symmetry of the Fe{211} surface (one mirror plane only) allows for the possible displacement of top atomic layers parallel to the surface as well as the more usual displacements perpendicular to the surface. The use of a large data base for our LEED experiment (30 *I–V* spectra, 19 non-equivalent, for three angles of incidence) coupled with the use of a reliability factor to measure quantitative agreement between theory and experiment has enabled the determination of the first three interlayer spacings and the registry shifts of the top two layers with an accuracy of 0.03–0.04 Å. The results of our analysis are: (i) an interlayer relaxation which alternates from 10% contraction to 5% expansion to 1% contraction, similar to recent results on Cu{110} and Al{110} and consistent with the pattern of recent theoretical calculations, (ii) a registry shift of the top Fe layer with respect to the second layer by an amount of 0.24 Å; this parallel shift of the first layer produces a more symmetrical relationship to the second layer as may well be a feature of less symmetrical surfaces than those commonly studied, and (iii) a registry shift of the second Fe layer relative to the third layer of 0.037 Å in the direction opposite to that of the first-layer registry shift.

The outline of the paper is as follows: § 2 describes sample preparation, cleaning procedures *in vacuo* and data collection; § 3 briefly details the dynamical LEED calculations used to generate theoretical *I–V* spectra. The final section is a discussion of the theory–experiment comparison and structure determination by means of reliability factor analysis.

2. Experimental details

The Fe{211} sample was spark-cut from a single-crystal specimen grown by strain-

annealing of ultra-pure source material provided by the American Iron and Steel Institute (for details see Shih *et al* 1980). The sample was oriented to within $\pm\frac{1}{2}°$ of the {211} plane with the aid of Laue photographs and then ground and mechanically polished with water-based alumina slurries (smallest bead size 0.3 μm).

Preparing a clean surface in ultra-high vacuum consisted of the following steps: (i) room-temperature argon-ion bombardment (2–4 μA at 400 eV) for 2 h, (ii) argon-ion bombardment with sample temperature raised to 850 °C for 2 h followed by 1 h anneal at same temperature, (iii) a series of argon-ion bombardments for 2–3 h with sample at 400–500 °C followed by 1 h anneal at 600–650 °C (total time of argon treatments approximately 25 h). Surface cleanness was monitored by Auger electron spectroscopy (AES), the main impurities before cleaning consisting of sulphur, carbon and oxygen. After cleaning, surface cleanness was similar to previous iron work (for example, Fe{111}, Shih *et al* 1981).

Thirty LEED intensity–energy curves (19 non-degenerate) were collected using a spot photometer, with the sample at room temperature for all measurements: 12 spectra at normal incidence ($10, \bar{1}0, 01, 0\bar{1}, 11, \bar{1}1, 1\bar{1}, \bar{1}\bar{1}, 20, \bar{2}0, 30$ and $\bar{3}0$), 11 spectra at $\theta = 7.1°$, $\varphi = 90°$ ($00, 10, \bar{1}0, 01, 0\bar{1}, 11, 1\bar{1}, \bar{1}\bar{1}, 0\bar{2}, 1\bar{2}$ and $\bar{1}\bar{2}$) and 7 spectra at $\theta = 10.7°$, $\varphi = 90°$ ($00, 10, \bar{1}0, 20, \bar{2}0, 1\bar{2}$, and $\bar{1}\bar{2}$). Angles and beam indices are given according to the convention of Zanazzi *et al* (1976). A schematic of the LEED pattern is shown in figure 1.

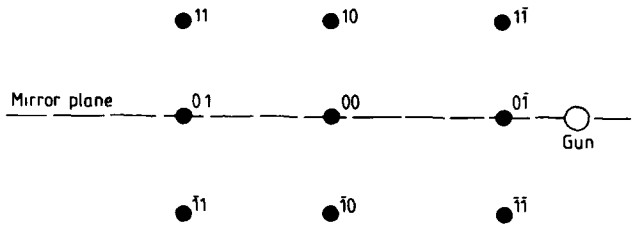

Figure 1. Schematic LEED pattern for clean Fe{211}.

3. Calculations

Dynamical intensity calculations were made using the THIN program described elsewhere (Jepsen 1980). The Fe potential was the same Hartree–Fock–Slater self-consistent potential used in previous Fe studies (for example, see Legg *et al* 1977). Both the real and imaginary parts of the inner potential were taken to be energy-independent. The imaginary part of the inner potential β was set at 4 eV and the real part V_0 was determined from the intensity analysis (initial value was −11.5 eV). Eight phase shifts and up to 55 beams were used to represent the electron wavefunction and the mean atomic vibrational amplitude was taken as $(\langle u^2 \rangle)^{1/2} = 0.115$ Å.

4. Structure analysis

A top view of the first two layers of an undistorted Fe{211} crystal is given in figure 2. The rectangular unit cell measures 4.05 Å along the ⟨110⟩ direction and 2.48 Å along the ⟨111⟩ (close-packed) direction. The surface structure is relatively open with a packing

fraction of 0.481. (The {110} surface of face-centred cubic crystals has a similar structure of close-packed rows separated by troughs formed with the second atomic layer. The packing fraction is 0.555. However, the FCC{110} surface has higher symmetry than the BCC{211} surface, as discussed below.) There are no rotational symmetries and the {110} plane is the only mirror plane. With the surface lattice vectors $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ as in figure 2 and $\boldsymbol{c}_{11}$ defined as the projection onto the {211} plane of the interlayer lattice vector, the

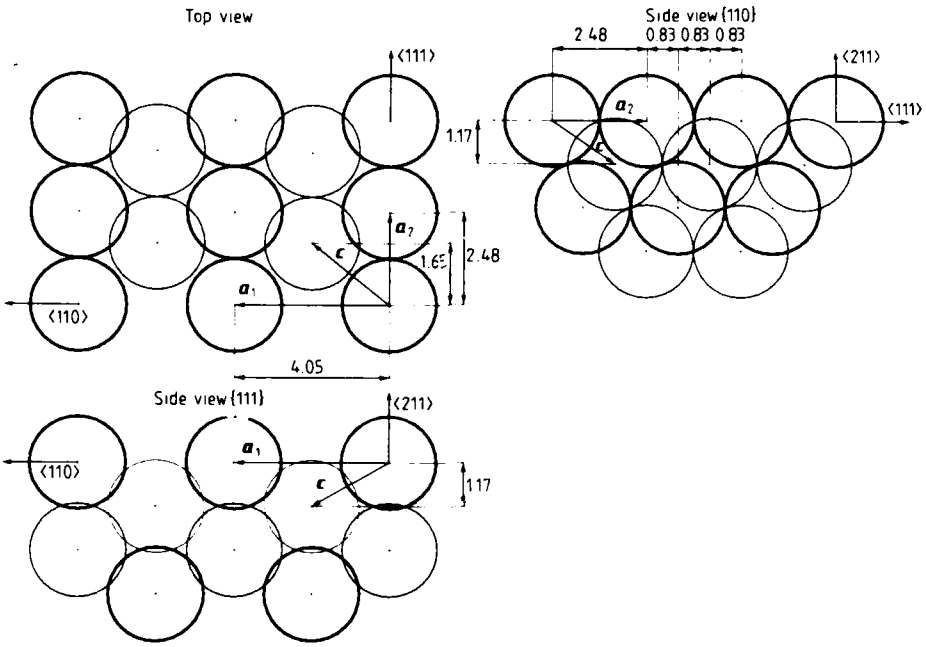

Figure 2. Atomic arrangement of undistorted Fe{211}.

bulk-like registry of the top layer with respect to the next layer is described by the relation $\boldsymbol{c}_{11} = \frac{1}{2}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_2$.

In contrast to the case of {100}, {110} and {111} surfaces with 1×1 structures the atoms in bulk-like positions on the Fe{211} surface are not symmetrically located with respect to the second-layer atoms. More precisely, a registry shift of the first atomic layer to the position described by $\boldsymbol{c}_{11} = \frac{1}{2}\boldsymbol{a}_1 + \frac{1}{2}\boldsymbol{a}_2$ (refer to figure 2) would cause each atom in the first layer to have four nearest neighbours in the second layer compared with only two for the bulk-like structure. However, such a motion would tend to *shorten* the nearest-neighbour distance between atoms in the first and third layers and *lengthen* the corresponding next nearest-neighbour distance as can be seen in figure 3. Because of the small distance between the first and third atomic layers (in a hard-sphere model of the bulk-like surface the two layers would be in contact) the influence of the third-layer atoms on any registry shift of the first layer is expected to be strong. The actual value of the registry shift, as well as values for relaxations of interlayer spacings, were to be determined by comparison of LEED spectra (I–V curves) with the calculations for the various structural models.

Preliminary calculations involved variation of the first interlayer spacings d_{12} for three models of the first-layer registry shift; (*a*) $\boldsymbol{c}_{11} = \frac{1}{2}\boldsymbol{a}_1 + \frac{1}{2}\boldsymbol{a}_2$ (henceforth called the

'$(\frac{1}{2}\,\frac{1}{2})$' model), (*b*) $\boldsymbol{c}_{11} = \frac{1}{2}\boldsymbol{a}_1 + \frac{7}{12}\boldsymbol{a}_2$ (the '$(\frac{1}{2}\,\frac{7}{12})$' model) and (*c*) $\boldsymbol{c}_{11} = \frac{1}{2}\boldsymbol{a}_1 + \frac{2}{3}\boldsymbol{a}_2$ (bulk-like model). Model (*a*) represents a registry shift of the top layer's close-packed atomic rows along a ⟨111⟩ direction (see figure 2) to a position where each first layer atom has four nearest neighbours in the second atomic layer as opposed to two for the bulk-like model (*c*). Model (*b*) consists of a registry shift half as large as for model (*a*). For each calculation, theory was compared with experiment using a reliability factor (Zanazzi and Jona 1977), including variation of the real part of the inner potential V_0. Results indicated that model (*a*) was noticeably worse than the others and it was rejected. Both models (*b*) and (*c*) gave fairly good agreement with experiment for d_{12} contracted $\approx 10\%$.

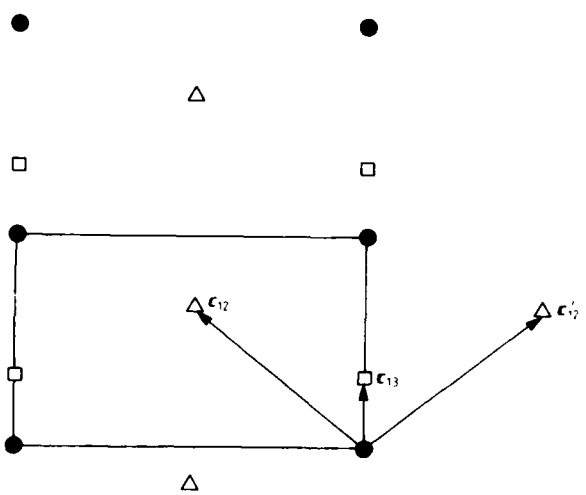

Figure 3. Schematic diagram of top three layers of Fe{211}. Full circles, first layer; triangles, second layer; squares, third layer.

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The next series of calculations involved varying the second interlayer spacing d_{23} while keeping d_{12} fixed at 10% contraction for both the $(\frac{1}{2}\,\frac{7}{12})$ and bulk-like models. The reliability factors (or *r*-factors) showed that the $(\frac{1}{2}\,\frac{7}{12})$ model had best agreement and that d_{23} was expanded by 5–10%.

Calculations were then made for independent variations of d_{12} and d_{23} for the $(\frac{1}{2}\,\frac{7}{12})$ model. Sixteen calculations were made in which d_{12} was varied from 1.01 Å to 1.09 Å (13.7–7% contraction) in steps of 0.026 Å, and d_{23} was varied from 1.20 Å to 1.28 Å (2.5–10% expansion) in steps of 0.026 Å. The *r*-factors for the calculations are shown in figure 4. The *r*-factors were fitted to a quadratic function of d_{12} and d_{23} (i.e. an elliptic paraboloid) to locate the *r*-factor minimum and corresponding best values for d_{12} and d_{23}. This procedure yields $d_{12} = 1.05$ Å and $d_{23} = 1.23$ Å. If the data sets for the three angles of incidence are considered separately, the results are: (*a*) $\theta = 0°$ (12 beams), $d_{12} = 1.05$ Å, $d_{23} = 1.23$ Å, (*b*) $\theta = 7.1°$, $\varphi = 90°$ (11 beams), $d_{12} = 1.05$ Å, $d_{23} = 1.24$ Å and (*c*) $\theta = 10.7°$, $\varphi = 90°$ (7 beams), $d_{12} = 1.04$ Å, $d_{23} = 1.24$ Å. The consistency is very good and is in fact better than our estimate of the inherent errors.

Next, calculations were performed varying the top-layer registry shift in the neighbourhood of the value for the $(\frac{1}{2}\,\frac{7}{12})$ model. The corresponding *r*-factors are shown in table 1 and it can be seen that the minimum lies very near to the registry shift of the $(\frac{1}{2}\,\frac{7}{12})$ model. A parabolic fit of the *r*-factors indicates that the best value of the shift is

0.24 Å away from the bulk position (the shift for the $(\frac{1}{2}\,\frac{7}{12})$ model is 0.21 Å). Because this optimum value of the shift, 0.24 Å, is very close to the value for the $(\frac{1}{2}\,\frac{7}{12})$ model, we did not make new calculations varying d_{12} and d_{23} although some correlation is to be expected.

We next considered variations of the registry shift of the second atomic layer with respect to the third layer for d_{12}, d_{23} and the first-to-second layer registry fixed at the

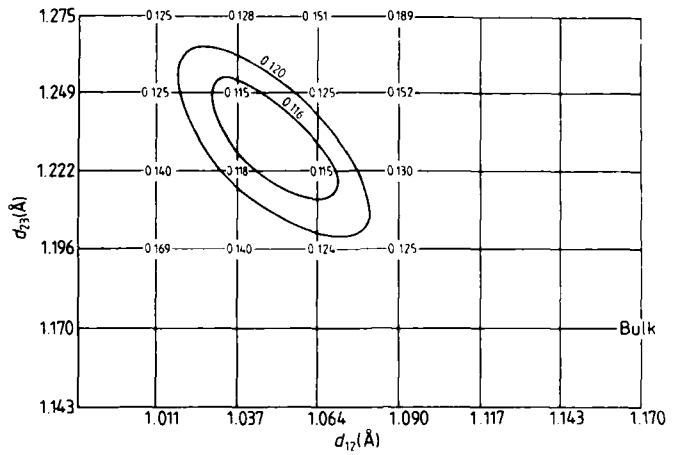

Figure 4. Values of reliability factor versus d_{12} and d_{23} for the $(\frac{1}{2}\,\frac{7}{12})$ model. $V_0 = -10.5$ eV. Contours for $r = 0.116$ and 0.120 are shown.

optimum values found above. Initial calculations showed that the second-to-third layer registry shift would be *opposite* to that of the first-to-second layer registry shift. For refinement of the shift value, calculations were performed for shifts of the second-to-third layer registry of 0.0 Å, 0.026 Å, 0.053 Å and 0.079 Å (or in notation similar to that used for the first-to-second layer registry: $(\frac{1}{2}\,\frac{2}{3})_{23}$, $(\frac{1}{2}\,0.68)_{23}$, $(\frac{1}{2}\,0.69)_{23}$ and $(\frac{1}{2}\,0.70)_{23}$ models respectively). The results are shown in table 2 and a parabolic fit to the r-factors yields a best value for the shift of 0.037 Å.

Lastly, we considered the possible deviation of the third interlayer spacing, d_{34}, from the bulk value of 1.17 Å. Calculations were made for variation of d_{34} over the range $1.12 \rightarrow 1.20$ Å steps of 0.026 Å with d_{12}, d_{23} and the registry shifts for the top two layers fixed at the optimum values given above. Table 3 shows the r-factors corresponding to variations in d_{34} and the real part of the inner potential V_0. Fitting the r-factors in table 3 to a quadratic function of V_0 and d_{34} indicates $V_0 = 11.3$ V and $d_{34} = 1.15$ Å (1.3% contraction) as best values.

It should be noted that the minimum r-factor for the calculation varying d_{34}, 0.116, is slightly higher than the minimum value of 0.111 for the calculations which did not vary

Table 1. Values of average r-factor for 12 beams (at $\theta = 0°$) for various models of first-layer registry shift with $d_{12} = 1.064$ Å, $d_{23} = 1.222$ Å and $V_0 = -10.5$ eV.

Model	$(\frac{1}{2}\,\frac{13}{24})$	$(\frac{1}{2}\,\frac{7}{12})$	$(\frac{1}{2}\,\frac{15}{24})$	$(\frac{1}{2}\,\frac{2}{3})$
r-factor	0.106	0.100	0.124	0.134

Table 2. Values of average r-factor for 30 beams for various models of second-to-third layer registry shift with d_{12} = 1.05 Å, d_{23} = 1.23 Å, first-to-second layer registry shift = 0.24 Å and V_0 = −10.5 eV.

Model	$(\frac{1}{2}\frac{2}{3})$	$(\frac{1}{2}0.68)$	$(\frac{1}{2}0.69)$	$(\frac{1}{2}0.70)$
r-factor	0.113	0.111	0.112	0.114

d_{34}. We believe this to be a computational effect due to the different ways of calculating the surface scattering. Calculations which include variations of d_{12}, d_{23} and d_{34} from their bulk values utilise a surface layer consisting of the top three atomic planes. The two-dimensional surface unit cell then contains three atoms and the multiple-scattering matrix for the entire surface layer of three atomic planes is calculated using the angular momentum (or spherical wave) representation. Scattering between the surface layer and the bulk is calculated in the beam (or plane wave) representation. In contrast, calculations which include variations of only d_{12} and d_{23} from their bulk values use a surface layer consisting of the top two atomic planes. The scattering matrix for the smaller surface layer is calculated in the angular momentum representation and scattering between the surface layer and the bulk is calculated in the beam representation. The observed trend, as measured by the r-factors, is that calculations using larger surface layers (i.e. more atoms per surface unit cell) are slightly less accurate. The effect is small but does give an indication of the size of calculational error arising from increasing the complexity of the unit cell. Although the exact cause of this error is uncertain, the *increased* use of the plane wave representation for the case of a smaller surface layer cannot directly account for the *correct trend* of smaller error for smaller surface unit cell since the transition to the plane wave representation involves the *approximation* of spherical waves by a finite number of plane waves.

Our analysis of the Fe{211} surface has determined optimal values for five structural parameters, d_{12}, d_{23}, d_{34} and the top two layer registry shifts, and one non-structural parameter, the real part of the inner potential V_0. The uncertainties associated with the given values of the parameters are complex (and unknown) functions of the various experimental and calculational errors and the method used to compare experiment with theory. Once a particular reliability factor (for example, see Zanazzi and Jona 1977, Pendry 1980, Van Hove *et al* 1977, Adams *et al* 1982) for measuring theory–experiment agreement has been chosen, there are essentially two approaches for extracting the *precision* (i.e. ignoring possible systematic errors) associated with the determination of the structural and non-structural parameters. (i) The curvature of the graph of the r-factor as a function of the parameters is used as a measure of sensitivity; graphs which

Table 3. Values of average r-factor for 30 beams versus d_{34} and V_0 with d_{12} = 1.05 Å, d_{23} = 1.23 Å, first-to-second layer registry shift = 0.24 Å and second-to-third layer registry shift = 0.037 Å.

d_{34} (Å)	V_0 (eV)		
	−12.5	−11.5	−10.5
1.196	0.201	0.153	0.129
1.170	0.162	0.126	0.119
1.143	0.135	0.116	0.127
1.117	0.125	0.125	0.153

show steep minima allow high precision for determination of the parameters (for example, see Adams *et al* 1982). (ii) The r-factor is used to determine the optimum values for all parameters for each I–V curve separately and the statistical mean and standard deviation of the parameter values for the set of all curves are calculated (for example, see Shih *et al* 1981). Also, the two methods can be combined. It should be emphasised that the uncertainties thus determined represent the precision and not the accuracy of the measurement of the given parameter. Because of possible systematic errors, the absolute accuracy of a LEED measurement is difficult to determine. Information from other surface techniques (EXAFS, UPS, ion scattering, etc) on the same structure would be useful for evaluating absolute accuracy.

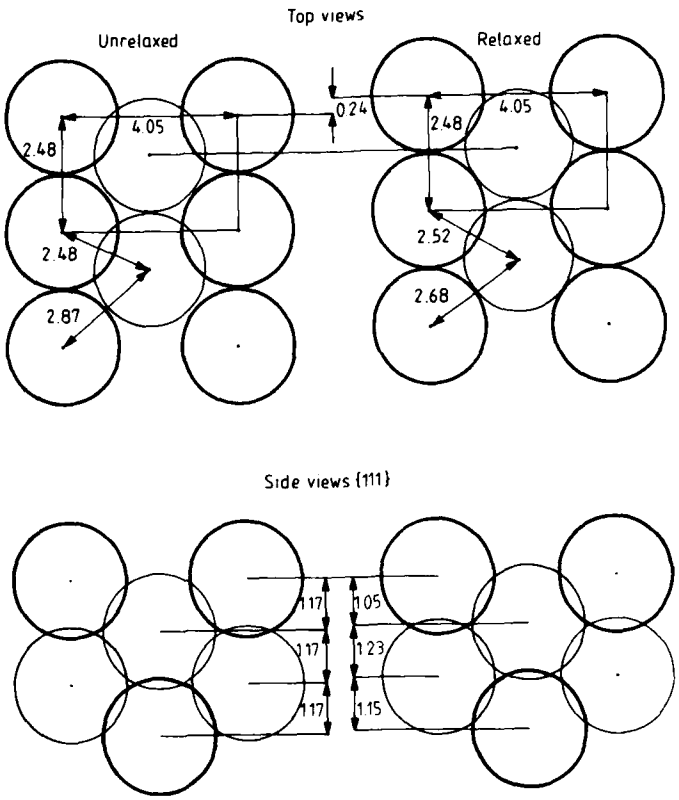

Figure 5. Top view of unrelaxed and relaxed surfaces of Fe{211} showing the first layer registry shift of 0.24 Å.

A recent paper (Moore *et al* 1982) compares the results of analysing LEED data from a Ni(311) surface using the r-factors of Zanazzi and Jona and of Pendry. The best value for the first interlayer spacing d_{12} of Ni(311) and the associated uncertainty (precision) were determined for three different definitions of the uncertainty. The agreement on the best value of d_{12} was very good; Pendry's r-factor indicated -13.5% contraction from the bulk value and Zanazzi and Jona's r-factor indicated -14.0% contraction. However, the error $\Delta d_{12}\%$ showed a substantial variation (from 1.2% to 4.2% corre-

sponding to 0.01–0.04 Å) depending on the choice of r-factor and method of fixing the uncertainty. In two cases where only the Zanazzi and Jona r-factor was used, Fe{110} (Shih *et al* 1980) and Fe{111} (Shih *et al* 1981) the authors give estimated errors of ±0.03–0.04 Å for the first interlayer spacings and ±0.4–1.1 eV for the real part of the inner potential V_0. In our analysis of Fe{211} the large number of structural and non-structural parameters and the expense of the LEED calculations has precluded a detailed error analysis as in the simpler cases cited above. We do believe those error values to be typical for LEED experiments and use them as guidelines for rather crude but reasonable error estimates for Fe{211}.

Summarising, the results of the LEED analysis are as follows:

first-to-second layer registry shift = 0.24 ± 0.03 Å (shift direction shown in figure 5)
second-to-third layer registry shift = 0.037 ± 0.03 Å (shift direction opposite to that of first)
d_{12} = 1.05 ± 0.03 Å ((10.4 ± 2.6)% contraction)
d_{23} = 1.23 ± 0.03 Å ((5.4 ± 2.6)% expansion)
d_{34} = 1.15 ± 0.04 Å ((1.3 ± 3.4)% contraction)
V_0 = −11.3 ± 0.5 eV (which agrees well with Fe{111} and Fe{110} values)
$\bar{r}_{min}$ = 0.111 (Zanazzi and Jona reliability factor).

The experimental and theoretical curves with the corresponding r-factors are shown in figure 6–8. A first-to-second layer registry shift of 0.41 Å would cause each top layer atom to have four nearest neighbours in the second layer compared with two for the bulk-like structure. The actual registry shift of 0.24 Å found from the LEED analysis represents a partial shift toward the 'quasi-fourfold' position as shown in figure 5. The pattern of damped oscillatory relaxation of the interlayer spacings from the bulk value is similar to that reported for experiments on Cu{110} (Adams *et al* 1982) and Al{110} (Nielsen *et al* 1982) and theoretical predictions for low-index faces of metals (Ma *et al* 1978, Landman *et al* 1980). However, in the case of surfaces such as Fe{211} which exhibit registry shifts as well as relaxations of interlayer spacings the pattern may not be general. Preliminary work on Fe{210} (Sokolov *et al* 1983) indicates a first-layer registry shift with d_{12} and d_{23} both contracted and d_{23} expanded. Further studies must be made before any regularities can be discerned.

It is interesting to compare our LEED results with the theoretical predictions of Johnson and White (1976). Using a short-ranged interatomic potential fitted to bulk elastic moduli (Johnson 1964), Johnson and White have calculated the surface relaxation of Fe{211}. The structure predicted by Johnson and White's model consists of negligible perpendicular relaxation, a first-to-second layer registry shift of 0.17 Å (73% of the observed LEED value) and a second-to-third layer registy shift of 0.049 Å (132% of the LEED value). Thus the registry shifts are at least partly accounted for while the perpendicular relaxations are greatly underestimated. Since the model did not include the important effects of surface electronic density redistribution (see e.g. Finnis and Heine 1974), which is expected to provide a substantial inward 'Madelung' force on the top layer, the underestimation of the perpendicular relaxation is not surprising. An approximate measure of the additional 'surface force' required for equilibrium can be obtained by calculating the net force on a top-layer atom due to the interatomic potential of Johnson when all iron atoms are taken to be in the positions of the fully relaxed structure determined by LEED. The calculated force has a component of 9×10^{-5} dyn along the outward surface normal and a component of 3×10^{-5} dyn parallel to the surface directed *opposite* to the first-layer registry shift (see figure 5). The force makes

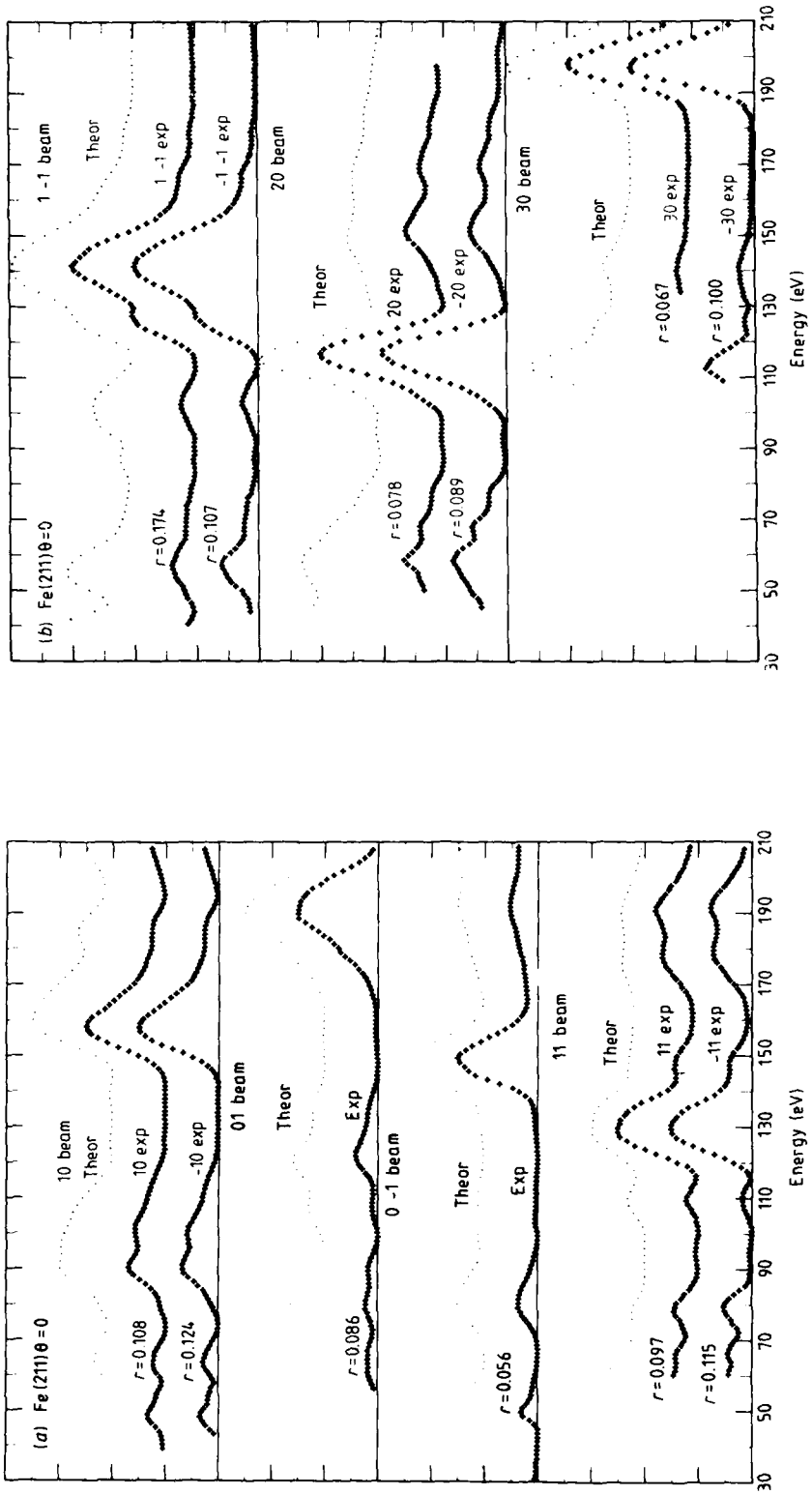

Figure 6. (*a*) and (*b*) Comparison of theoretical and experimental intensity spectra for Fe(211) $\theta = 0$. Best-fit values for structural parameters are: $d_{12} = 1.05$ Å, $d_{23} = 1.23$ Å, $d_{34} = 1.15$ Å, first-to-second layer registry shift = 0.24 Å and second-to-third layer registry shift = 0.037 Å, $V_0 = -11.3$ eV and $\beta = 4$ eV. Intensities of the largest peaks in each curve are normalised to the same value.

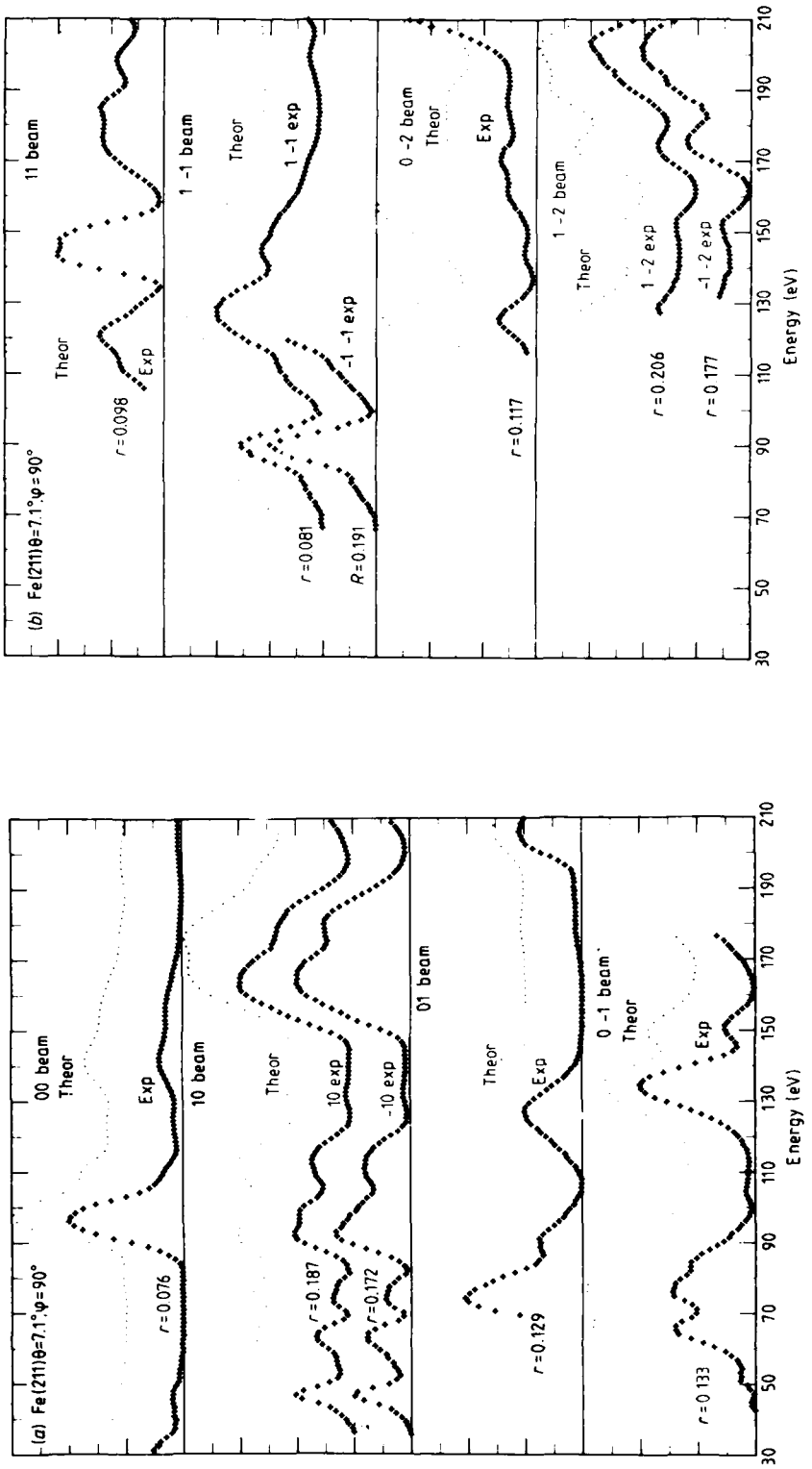

Figure 7. (*a*) and (*b*) Same as figure 6 but for $\theta = 7.1°$, $\varphi = 90°$.

an angle of 18° with the surface normal. To maintain equilibrium, the additional 'surface force' would have to be of equal magnitude and opposite direction, i.e. into the surface but with a non-zero parallel component.

Any quantitatively reliable theory of iron surface relaxations must accurately account for surface electronic density redistribution. This will be more difficult for the transition metals such as iron than for the simple metal aluminium but we hope that our results on Fe{211} will generate new interest.

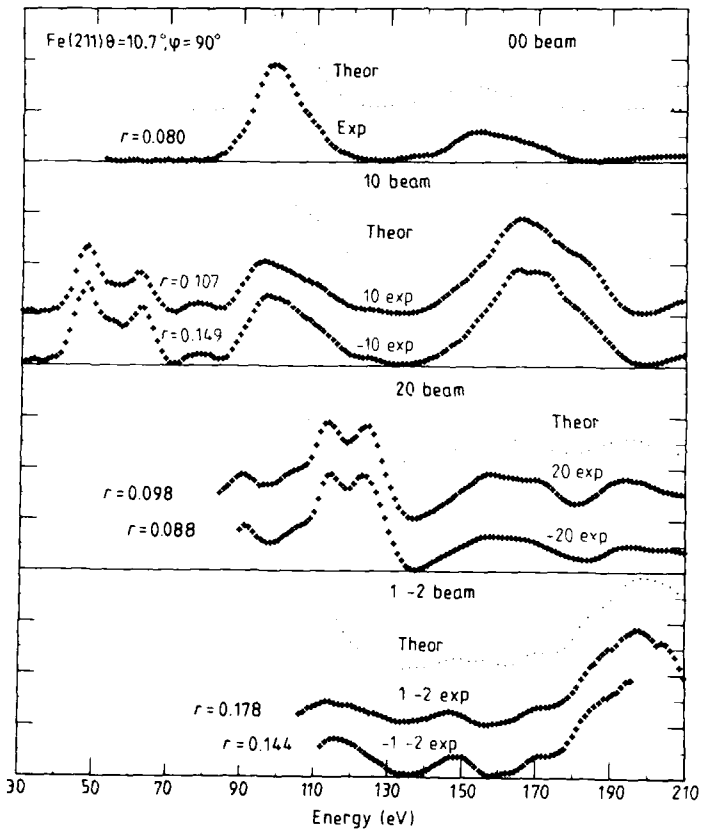

Figure 8. Same as figure 6 but for $\theta = 10.7°$, $\varphi = 90°$.

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