Iron multilayers on Cu(100) – a case of complex reconstruction investigated by quantitative LEED

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Abstract

Epitaxial growth of iron on Cu(100) leads to the formation of fcc iron whereby as function of film thickness a variety of different structures is observed. As detected by full dynamical LEED structure analyses using tensor LEED these structures are rather complex. In the coverage regime below 5 monolayers all iron layers are reconstructed both vertically and in-plane. Above 5 monolayers only the top layer is reconstructed until a martensitic transformation at about 10 monolayers leads to the formation of a bcc(110) surface. The structures found correlate nicely with known magnetic properties. Surprisingly, the in-plane lattice parameter of the fcc iron layers was found to be 2.52 Å, i.e. smaller than the value of 2.55 Å known for bulk copper layers. However, a re-investigation of clean Cu(100) also yields a 1% in-plane contraction of copper surface layers compared to bulk layers, i.e. the clean copper surface – at least after conventional preparation procedures – relaxes under its surface stress. In conclusion, the growth of Fe on Cu(100) has to be regarded as pseudomorphic.

Keywords: Copper; Epitaxy; Iron; Low energy electron diffraction (LEED); Metallic films; Surface relaxation and reconstruction; Surface tension

1. Introduction

The epitaxial growth of iron on copper is most interesting by several points of view. First and as well known, in a certain coverage regime fcc iron (γ-Fe) can be grown at room temperature or below. This structural phase of iron is stable by itself only at higher temperatures, namely between 1185 and 1667 K. Second, the magnetization of these fcc iron films is normal to the surface independent of film thickness. This, at least in principle, is interesting also from the application point of view. Third, there seems to be a direct and intrinsic relation between the structural details and the magnetic properties of the films, which both vary considerably with film thickness. Corresponding accurate experimental data are extremely valuable as input to theory in order to allow for a deeper and experimentally confirmed understanding of the correlation between structure and magnetism. Last but not least, it is of interest how the iron atoms accommodate to the copper substrate, in particular whether or not they take the substrate’s lattice parameter, i.e. whether there is pseudomorphic or non-pseudomorphic growth. We will see that by surprising new results for the in-plane lattice parameter of the clean copper surface, the

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growth of iron has to be concluded as pseudomorphic.

The present paper is organized as follows: In the next section a survey about the rough structural and magnetic properties of Fe/Cu(100) as appearing by low energy electron diffraction (LEED) patterns and surface magneto-optical Kerr effect (SMOKE) data as taken from Ref. [1] are given for phases of different film thicknesses. In Section 3 the crystallographic structure of the different phases as resulting by detailed LEED analyses are presented and discussed in connection with the corresponding magnetic properties. Section 4 deals with the question of pseudomorphic or non-pseudomorphic growth and its result leads to Section 5, which presents a new high precision LEED analysis with emphasis on the in-plane reconstruction of clean Cu(100). All results are summarized in the final paragraph.

2. Structural and magnetic phases of epitaxial Fe/Cu(100)

The simplest model to imagine the epitaxy of Fe on Cu(100) would be a layer-by-layer growth whereby iron just continues the fcc arrangement of substrate atoms with simultaneous adoption of their lateral lattice parameter. This persuasive model is favoured by the fact, that the lattice parameter of the high temperature fcc iron phase when extrapolated to low temperatures falls — dependent on which thermal expansion coefficient is used — into the range 3.55–3.58 Å. This is very near the value of copper \( a(\text{Cu}) = 3.61 \) Å so that iron can be expected to make up with the small mismatch of 1–2%. Then, from the structural point of view the continuation of the substrate’s lattice would be rather unspectacular. The geometry of the LEED pattern would stay unmodi-

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Fig. 1. Dependence of the SMOKE signal on Fe coverage on Cu(100) (counted in monolayers (ML)) and appearance of LEED patterns at certain coverage values.
fied and intensity spectra would – if ever – exhibit only some peak shifts due to modified interlayer spacings. Concerning the magnetic properties, the magnetization as recorded by SMOKE experiments should just increase linearly with coverage because each new layer would just add its magnetic moment to the signal of the film below.

However, the epitaxial growth of Fe on Cu(100) is everything else than that simple. As demonstrated by the scenario displayed in Fig. 1 for iron deposition at room temperature superstructure spots appear in the LEED pattern at almost every coverage indicating that at least one of the iron layers in each case must be reconstructed. Practically all patterns show a substantial amount of background indicating that the long range order in the films is far from ideal. At about 10 ML a rather complex diffraction pattern develops which, as will be demonstrated below, is due to a phase transition of the film to the thermodynamically stable bcc(110) phase arranged on the fcc(100) substrate. As displayed by the graph in Fig. 1 (taken from Ref. [1]) the magnetic properties are of similar complexity as the structural behaviour. The SMOKE signal is by no means uniform but exhibits a pronounced dependence on coverage (see also Refs. [2,3]). Obviously this is correlated with the structural properties.

At low coverages there is a strong magnetization with an almost linear increase with coverage until a strong decrease takes place at and above about 4 ML. The increase is indicative for the ferromagnetic coupling of layers so that with each layer (or atom) added the signal increases by a constant amount. The structures of the films in this regime seem – according to the diffraction patterns – to be very similar, though not simple. Superstructure beams appear at 1/4-order positions for 2 ML coverage and at 1/5-order positions for 4 ML. However, as obvious from the patterns shown, extra spots with detectable intensity show up only in the immediate neighbourhood of substrate spots, i.e. as their satellites. This feature will be of help for the selection of the correct structural models.

At intermediate coverages (5–10 ML) the Kerr signal is almost constant and remains at a comparably low level. In this regime, the symmetry of the diffraction pattern transforms to (2 × 1)\textsubscript{p2mg} (denoted 2 × 1 in Fig. 1 for simplicity reasons). Half-order spots are missing on the unit mesh axis indicative for the existence of glide symmetry planes. Whilst the extra spots are intense and sharp at about 6 ML, they gradually disappear with further increasing coverage with a simultaneous increase of background intensities. It will be shown below by comparison of discrete beam and diffuse intensity data that the local structure, i.e. the reconstruction in this coverage regime is constant and only long range order gradually disappears. The described coverage regime ends at about 10 ML with the breakdown and subsequent re-increase of the SMOKE signal accompanied by the development and further growth of the bcc(110) phase.

3. Structure determination by quantitative LEED

3.1. Experimental and computational basics

The structures of all phases displayed in Fig. 1 have been analyzed by the measurement and quantitative analysis of their LEED intensities. LEED is one of the very few techniques which provide the full structure of a surface rather than only special structural features as e.g. bond lengths or positions of only top layer atoms. This unique property has to be paid for by a considerable complexity of the numerical intensity analysis for which the multiple scattering of low energy electrons has to be taken into account. Eventually, coordinates and some non-structural parameters as e.g. vibrational amplitudes result in a surface slab of atoms whose vertical size is determined by the electron attenuation.

The iron films were deposited at room temperature by evaporation from a reservoir of 4N purity [4] under the control of Auger electron spectroscopy and a crystal microbalance. The LEED measurements were performed using a video based technique operated under computer control as described in detail elsewhere [5,6]. The method works by enframing the spot under consideration by an electronic window which follows the beam with sweeping energy. At each energy the intensities within the window are integrated and the background determined at the window's edges is subtracted automatically. Spectra result with a maximum rate of 1 intensity versus energy point per video half frame (20 ms). Though
this procedure works perfectly for well-separated spots it is not easily applicable to spots close to each other as e.g. the spots in the above $4 \times 1$ superstructure. In this case, with strong substrate spots and weak extra spots neighboured, the intensities were taken by measuring spatial profiles through the spots with subsequent integration and background subtraction “by hand” [7]. Though this procedure is tedious it produces reliable data because the intensity profiles can be taken with high speed, i.e. the video rate. Only the off-line evaluation is slow. All measurements were taken at normal incidence of the primary beam and at 90 K. Symmetrically equivalent beams were averaged in order to improve the quality of the data and to reduce the influence of residual sample misalignment.

The intensities were calculated full dynamically according to certain structural models. For the comparably simple structures in the regime $> 5$ ML the use of standard computer programs was sufficient [8,9]. However, the determination of the complex $4 \times 1$ and $5 \times 1$ reconstructions could only be realized by the application of the perturbation method tensor LEED which allows the fast calculation of intensities for structures differing by only small displacements of atoms [10–12]. The parameter space was scanned conventionally in order to find the best theory–experiment fit whereby vertical coordinates were adjusted prior to in-plane parameters, a procedure which was iterated until convergence was achieved. The Pendry $R$-factor, $R_p$, [13] was used for the quantitative comparison of experimental and calculated data.

3.2. Coverage dependent film structures

The structural models found for the various phases are displayed in on-top and side views in Fig. 2 together with their schematic diffraction patterns above (the structure labelled (5) in Fig. 1 is omitted.

![Diffraction patterns and structural models]

Fig. 2. Schematic diffraction patterns (top row) and structural models in on-top (middle) and side (bottom) views for the different adsorption structures.
because it shows the same local structure as structure (4). Extra spots extincted by symmetry are indicated by open symbols. In the on-top views only the top substrate layer (open circles) and the top iron layer (shaded) are displayed for simplicity reasons. The side views display all iron layers in each case with again only the top copper layer.

As already mentioned the 4 × 1 and 5 × 1 structures are peculiar in the sense that extra spots appear only when neighboured to substrate spots. This dramatically reduces the number of possible models in both cases [1,7]. Eventually and as speculated quite early [14], laterally sinusoidal-like distorted iron layers as indicated in Fig. 2 account for the observed extinction of most extra spots. In order to obtain a satisfying fit between experimental and model spectra, all iron layers have to be allowed to reconstruct. Moreover, the reconstruction has to be both in-plane and vertical to the ideal plane. Eventually, for each of the 4 (5) atoms in the 4 × 1 (5 × 1) unit cell two coordinates must be determined (note that one in-plane coordinate is fixed because the reconstructions consists of mutual shifts of complete atomic rows). For the 5 × 1 phase with 5 inequivalent atoms in each of the four layers this amounts to the determination of as much as 40 coordinates. This was done by the use of tensor LEED with an only in-plane and strictly sinusoidal reconstruction identical for all iron layers as reference structure [15]. A similar procedure was applied for the 4 × 1 phase. The resulting best fit parameter values are given in the first two columns of Table 1 whereby for the atomic displacements off the ideal fcc sites only the maximum values si (in-plane shift) and bi (vertical buckling) for each layer i are given for simplicity reasons (for more details see Ref. [15]). Apparently, the layer reconstructions are accompanied by a substantial expansion of iron interlayer distances di,i+1 (measured with respect to the centre of mass planes) compared to the ideal fcc bulk distance of 1.78 Å. This holds both for the 4 × 1 and 5 × 1 phase and yields an increased atomic volume for iron atoms in all layers of these structures. In turn this is in agreement with the ferromagnetic properties of the films in the corresponding low coverage regime: as proved by first principle calculations in the local spin density approximation the observed increased atomic volume is consistent with the ferromagnetic coupling of atoms in the film [16–18]. Therefore, as demonstrated in Fig. 1 the SMOKE signal increases steeply and linearly with coverage in the low coverage regime.

In the medium coverage regime (5–10 ML) the complex multilayer reconstruction is lifted. At around 6 ML a sharp superstructure with (2 × 1)p2mg symmetry appears as displayed in Fig. 1. The structure analysis shows that reconstruction of subsurface layers has vanished with the interlayer distances relaxed to the equilibrium value (Table 1). Only the top layer remains reconstructed with a sinusoidal (or zig-zag) in-plane reconstruction with 2-fold periodicity and amplitude 0.20 Å. Its glide symmetry plane accounts for the extinction of extra spots on the unit mesh axis. With increasing coverage the extra spots gradually disappear under simultaneous development of

<table>
<thead>
<tr>
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<th>2 ML</th>
<th>4 ML</th>
<th>6 ML</th>
<th>8 ML</th>
<th>12 ML</th>
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<tbody>
<tr>
<td>d12 (Å)</td>
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<td>1.86</td>
<td>1.87</td>
<td>1.87</td>
<td>2.00</td>
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<tr>
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<td>1.90</td>
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<td>1.78</td>
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<tr>
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<td>1.85</td>
<td>1.76</td>
<td>1.76</td>
<td>1.99</td>
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<tr>
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<td>1.78</td>
<td>1.77</td>
<td>2.03</td>
<td></td>
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<tr>
<td>b1/s1 (Å)</td>
<td>0.18/0.5</td>
<td>0.28/0.4</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
</tr>
<tr>
<td>b2/s2 (Å)</td>
<td>0.04/0.3</td>
<td>0.11/0.3</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
</tr>
<tr>
<td>b3/s3 (Å)</td>
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<td>0.12/0.3</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
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<tr>
<td>b4/s4 (Å)</td>
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<td>0.21/0.4</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
<td>&lt;0.20/0.16</td>
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<tr>
<td>R_p</td>
<td>0.18</td>
<td>0.14</td>
<td>0.11</td>
<td>0.09</td>
<td>0.13</td>
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</table>

The dik stand for the distances between the centre of mass planes of layers i and k. The quantities bi and si represent the maximum vertical and lateral atomic shifts, respectively, in the i-th iron layer. R_p represents the Pendry R-factor for the best theory–experiment fit.
background intensities. This indicates that there is no simple transformation to a $1 \times 1$ phase, but only long range order of the $2 \times 1$ reconstruction is lifted. In fact, if diffuse intensities are taken at the very positions of the $2 \times 1$ fractional-order spots they compare very well to the spectra of discrete beams (Fig. 3). This proves that the local structure in both phases is the same, i.e. in the whole coverage regime 5–10 ML the surface is at least locally reconstructed according to the model given in Fig. 2 for the 6 ML coverage. In fact, the analysis of both the ordered and disordered phases yield practically the same parameters as given in Table 1. Only the top layer distance is increased according to the surface reconstruction, whilst subsurface layers are ideally flat with a relaxed interlayer distance. So, there is ferromagnetism only in the very surface region whilst the bulk of the film is antiferromagnetic [1]. This nicely correlates with the low and coverage independent SMOKE signal displayed in Fig. 1.

At about 10 ML the near fcc arrangement of iron atoms becomes unstable and the whole film transforms to bcc(110). There are four symmetrically equivalent arrangements of bcc(110) domains on the fcc(100) substrate leading to the total of observed spots (the reciprocal unit mesh of one domain is displayed in Fig. 2). The measurement and analysis of their intensities [19] proves the existence of a slab of iron layers with essentially the same structure as the (110) surface of a Fe single crystal. This is demonstrated by the interlayer distances retrieved for a 12 ML film given in Table 1 which almost exactly compare to the parameters determined for the (110) iron crystal surface [20–22]. This is consistent with a martensitic transition, for which the zig-zag reconstruction in the $(2 \times 1)_{\text{zig}}$ phase might be a precursor. Upon the transition fcc $\rightarrow$ bcc the surface magnetization changes from vertical to in-plane and the SMOKE signal again starts to increase with film thickness due to ferromagnetism in the entire film (Fig. 1).

4. Pseudomorphic versus non-pseudomorphic growth

Up to this point the question whether the growth of fcc iron on Cu(100) is pseudomorphic or not remained unaddressed because we simply assumed that iron atoms adopt the in-plane primitive lattice parameter of bulk Cu(100) layers which is $a_p(Cu) = 2.55 \, \text{Å}$. This assumption seemed to be justified by the very similar value applying for fcc iron extrapolated from the high temperature fcc iron phase yielding $a_p(Fe) = 2.51–2.53 \, \text{Å}$ dependent on the exact thermal expansion coefficient used. The iron layers should easily make up with an expansion by about 1%. However, by applying $a_p(Fe) = 2.55 \, \text{Å}$ we found some strange value of the inner potential, which with $V_{\text{cr}} = 7.5 \, \text{eV}$ is far too low. We took that as a hint for a possibly wrong in-plane lattice parameter and tried to check for the correct value of $a_p$.

Unfortunately, an in-plane parameter contracted by only 1% compared to the substrate value would not easily be visible in the LEED pattern because of the finite width of the LEED spots due to the finite electron coherence length (typically 100 Å $\approx$ 40 lattice parameters). The only chance comes by the evaluation of intensity spectra with respect to $a_p$. However, intensity spectra are dominated by parameters vertical to the surface and usually there is less sensitivity to surface parallel parameters. Yet this sensitivity comes back if the theory–experiment fit is close enough so that small changes in the spectra become of influence. Therefore, we chose the 8 ML film for which for $a_p(Fe) = 2.55 \, \text{Å}$ we had reached a minimum $R$-factor of $R_p = 0.14$. Also, for this film thickness the underlying copper substrate has very little or no influence on the spectra because of electron attenuation and so there is no difficulty with incommensurable structures. We reanalysed this
phase and additional to the variation of the first three interlayer distances \(d_{i,i+1}\), the constant distance \(d_b\) of layers below, the top layer reconstruction amplitude \(s_1\) and the surface Debye temperature \(\Theta_0\), the in-plane lattice parameter \(a_p\) was varied. Fig. 4 displays the \(R\)-factor behaviour as function of \(a_p\) with all other parameters optimized for each value of \(a_p\). The best fit is for \(a_p = 2.52 \pm 0.015 \ \text{Å}\) whereby the error limits result by the variance of the Pendry \(R\)-factor [13]. The inner potential now turns out to have a much more reasonable value, i.e. 11.5 eV. The best fit values of the other parameters are given in Table 1 which is based on \(a_p = 2.52 \ \text{Å}\) in order to avoid confusion by too many parameter values. The bulk interlayer distance is \(d_b = 1.77 \pm 0.015 \ \text{Å}\) which is very near the value \(d_b = a_p/\sqrt{2}\).

Clearly, the copper bulk value of 2.55 Å is ruled out and on the first sight one is inclined to conclude non-pseudomorphic growth of iron [23]. However, though \(a_p = 2.52 \ \text{Å}\) nicely corresponds to the equilibrium value of fcc iron, it is hard to believe that the film cannot accommodate to the substrate by an expansion as low as 1%. Additionally, for the epitaxial system Ni/Cu(100) we found a value of \(a_p = 2.53 \ \text{Å}\) for the lattice parameter [24,25] which nearly coincides with the value of the Fe films, though the equilibrium value of nickel is 2.49 Å. Both findings could be easily explained by an in-plane lattice constant of copper smaller at its surface as compared to the bulk. Therefore, we reinvestigated the structure of the clean Cu(100) surface with emphasis on the determination of \(a_p\), which normally is not varied in a structure analysis but assumed to exhibit the bulk value.

5. In-plane lattice contraction of clean Cu(100)

Because of the restricted sensitivity of normal incidence LEED data with respect to surface parallel parameters much care was taken to achieve both reliable experimental data and their reliable full dynamical analysis [26]. Data for 5 inequivalent beams were measured at 90 K with a total energy width of 1600 eV. Normal incidence was chosen because it can be adjusted with much higher precision than for oblique incidence (yet, an oblique incidence analysis is in progress). The measurements were reproducible within an \(R\)-factor level of \(R_p < 0.02\). A total of 15 phase shifts calculated relativistically with eventual spin averaging were used. They were corrected for thermal vibrations using the bulk Debye temperature (443 K) for subsurface layers and a variable fit value for the surface layer. Additional to \(a_p\) the first 6 interlayer spacings \(d_{i,i+1}\) and the constant spacing \(d_b\) of deeper layers were varied independently in steps of 1/100 Å.

The variation of the Pendry \(R\)-factor as function of \(a_p\) with all other parameters optimized for each \(a_p\) is displayed in Fig. 5. Clearly, the absolute minimum develops below the bulk value (vertical line),

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**Fig. 4.** \(R\)-factor behaviour as function of the in-plane lattice constant \(a_p\) for the 8 ML film with all other parameters optimized for each value of \(a_p\).**

**Fig. 5.** Variation of the Pendry \(R\)-factor for Cu(100) with varying in-plane lattice parameter \(a_p\), i.e. nearest neighbour distance. For each value of \(a_p\) all other parameters are optimized. The horizontal line indicates the level of the \(R\)-factor variance, the vertical line corresponds to the bulk value of \(a_p\).
i.e. for about 1% in-plane contraction at \( a_p = 2.53 \) Å. There is excellent theory–experiment agreement according to a Pendry R-factor of \( R_p = 0.085 \) (the also applied relative mean square deviation between experimental and best fit intensities is \( R_2 = 0.018 \)). The error limits for \( a_p \) as taken from the variance of the Pendry R-factor are ±0.01 Å, i.e. the deviation from the bulk value is outside the limits of error. However, this error estimation is on the basis of only statistical errors and does not account for systematic errors which might show up at the very low R-factor level reached. Therefore, as general test we applied the same procedure of determining \( a_p \) for another surface. We chose the substitutionally disordered alloy surface Mo\(_{75}\)Re\(_{25}\)(100) because for this surface we had obtained a low R-factor before [27] which, as pointed out above, is essential to provide the necessary sensitivity with respect to an in-plane structural parameter. The analysis yields \( a_p = 3.125 ± 0.01 \) Å \((R\)-factors \( R_p = 0.117, R_2 = 0.030\) in perfect agreement with the bulk value \( a_p = 3.127 \) Å [28,29]. This proves that our analyses do not suffer from some built in errors in experiment or theory which automatically would produce an in-plane lattice contraction. We also checked for systematic errors as possibly imposed by e.g. the influence of inaccurate phase shifts, an energy dependent inner potential or the presence of mosaic structures on the sample. However, all these error sources turned out not to account for the observed contraction [26].

The in-plane contraction detected for Cu(100) entails that the growth of iron on this surface is pseudomorphic. Obviously, the surface gives way to the tensile stress present at any surface. This is consistent with an earlier investigation of Cu(100) where the Raleigh phonon dispersion had been explained by either a modified force constant between the first and second layer or a “tendency of the surface layer to contract” [29]. An in-plane contraction is observed also for other surfaces, as e.g. the (100) surfaces of Pt, Ir and Au. Yet, their contraction even breaks the original surface symmetry and – different from the present cases – is substantial enough to cause the appearance of extra spots in the LEED patterns. However, these surfaces can be prepared also in metastable \( 1 \times 1 \) phases and we have reanalysed with respect to \( a_p \), corresponding data measured earlier for Pt(100) \( 1 \times 1 \) [30]. We find again a 1% contraction although according to ab initio calculations Pt should exhibit a higher surface stress than Cu [31] and thus a larger contraction should be expected. However, the extent by which a surface gives way to its surface stress via some in-plane contraction depends on a delicate balance between energy gain and cost caused by the stress release and developing mismatch, respectively [31]. Also, the contraction requires the formation of defects as possibly steps or grain boundaries and it might be that such defects are induced during the sample preparation. If a surface without any defects could be prepared, there should be, of course, no in-plane contraction.

6. Summary

As demonstrated, the growth of iron on Cu(100) is everything else than a simple continuation of the substrate by adding flat fcc(100) iron layers. More or less the whole system is reconstructed. Starting with the clean substrate, whose surface is also different from bulk termination by a small in-plane contraction, the first few iron layers up to 4 ML deposited at room temperature are reconstructed by both substantial in-plane and vertical atomic displacements compared to undistorted fcc(100) layers. This leads to an increased atomic volume in the whole film which is consistent with the observed ferromagnetism. Above 4 ML coverage all iron layers flatten and only the top layer keeps to exhibit a zig-zag in-plane reconstruction. Consistently, ferromagnetism concentrates to the very surface whilst the bulk of the film becomes antiferromagnetic. The in-plane lattice constant of 2.52 Å is within the limits of error the same as detected for the (contracted) clean substrate and coincides with the equilibrium value of fcc-iron as extrapolated from its high temperature phase. At about 10 ML the fcc iron film becomes unstable and in a martensitic transition transforms to a bcc(110) film which is structurally identical to clean Fe(110).

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