Manipulation and control of the growth of magnetic iron nitride films
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Chapter 5. Mechanism of growth of Fe₄N on MgO(100)

5.1. Introduction

As was shown in Chapter 3, the MBE growth assisted with a flow of atomic nitrogen from a RF-source is an effective method for the production of the pure γ'-Fe₄N phase. However, many questions about the growth mechanism remained open. For instance, the role of hydrogen and the fact that the growth of an epitaxial phase takes place on a substrate with a lattice mismatch of 10%. The growth mechanism is an interesting subject in itself. It involves many surface processes like sticking, adsorption, surface diffusion, chemisorption, nucleation, decomposition of a phase, recombination, and more. In our system, Fe, N and H atoms participate in these processes at surfaces of the substrate, or of an iron nitride, or of pure iron. This makes the picture very complex and intricate. We hope to get more insight in the mechanism by breaking up the whole process into a number of simpler sub-processes. One such a sub-process is the sticking of N atoms to an iron or iron nitride surface. Also the role of hydrogen in surface processes and in the RF-source will be discussed in this chapter. A series of samples was produced in order to characterize the mentioned processes. Table 1 gives an overview of the samples grown. All samples were grown at a substrate temperature of 350°C with the exception of sample 1, which was grown at room temperature. The CEMS spectra were fitted with four sextets representing the α-Fe (one sextet) and γ'-Fe₄N (three sextets) phases and with a nonmagnetic doublet. This nonmagnetic component is present in each sample we grow and is attributed to a surface layer, which has reacted with air [1, 2]. The thickness of the samples was measured with RBS and was about 250Å for all samples. Our observations will lead us to a tentative model of the growth of Fe₄N on a MgO(100) substrate.

5.2. Sticking coefficient of N atoms to iron

The probability for a particle hitting a surface to stick and then to be incorporated into the growing film is known as a sticking probability. The sticking coefficient is an important item in all chemisorption processes. It determines the rate of the reaction at the surface and defines the fluxes needed to obtain a certain composition of the deposited layer. When the sticking coefficient is smaller than unity it will obviously depend on the substrate temperature. It can be argued that, with a large probability, the sticking coefficient must be equal to unity (if not zero) when it does not depend on the substrate temperature. In this spirit we have grown two Fe-N samples at room temperature and at 350°C leaving the other growth conditions identical. We have chosen the growth rate of iron to be 0.06 Å/s for both samples, which in combination with a certain flux from the RF-source would result in an insufficient amount of nitrogen for the formation of pure Fe₄N.

The two samples grown had very different crystalline properties (table 5.1, samples 1 and 2). The CEMS of the sample grown at the higher temperature showed sextets of α-Fe and
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γ′-Fe₄N (figure 5.1b). We observed channeling dips in this sample, which implies the formation of an epitaxial layer. The off-specular XRD θ-2θ scan contained no peaks, whereas the specular spectrum showed very pronounced peaks of the two phases. This confirmed that the two mentioned phases were both epitaxial (figure 5.1d). The CEMS spectrum of the sample grown at room temperature consists of broad sextets of iron and of a few other magnetic components, with hyperfine parameters not corresponding to any known iron nitride phase (figure 5.1a). The presence of broad peaks in the spectrum points at a distribution of iron atoms with slightly different surroundings. The peaks in the XRD scans were also very broad, and appeared at positions of the (002) reflection from α-Fe and the (002) reflection from α′-Fe₄N (see figure 5.1c). The width of these reflections corresponds to a crystallite size of the order of 3-4 nm assuming that the width can be fully explained by Scherrer broadening [3]. The XRD scan taken with an offset of 6° showed no peaks at all, suggesting a strong texture in the film (figure 5.1c). However, from the analyses of both RBS and ERD experiments we determined that the content of nitrogen was the same in both cases. A small difference in results obtained by RBS+CEMS versus ERD is due to a systematic error in the estimation of the nitrogen content by RBS and CEMS. The RBS technique is relatively insensitive to light elements, and while deriving the N content from CEMS spectra we had to assume a certain nitrogen content of the extra phase, which is due to oxidation. Still both RBS+CEMS and ERD each give an equal amount of nitrogen in both samples within the estimated uncertainty.

An obvious way to explain this result would be that the sticking coefficient of atomic N to a growing Fe and/or Fe-N layer is very close to unity in the temperature range investigated. In case of higher fluxes of N, when the amount of N atoms will be more than enough for the formation of Fe₄N, the sticking coefficient might decrease because further nitridation of the growing layer will include a phase transformation into the ε phase or another iron nitride with a higher concentration of nitrogen.

<table>
<thead>
<tr>
<th>Evaporation rate of ⁵⁷Fe, Å/s</th>
<th>RF-source gas</th>
<th>External H₂, mbar</th>
<th>CEMS results in %, Fe:Fe₄N:non-magnetic</th>
<th>uptake of N, x10¹² at/s</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.064</td>
<td>N₂</td>
<td>nano-crystalline</td>
<td>(7.4)</td>
</tr>
<tr>
<td>2</td>
<td>0.062</td>
<td>N₂</td>
<td>-</td>
<td>48:38:14</td>
</tr>
<tr>
<td>3</td>
<td>0.025</td>
<td>N₂</td>
<td>-</td>
<td>17:72:11</td>
</tr>
<tr>
<td>4</td>
<td>0.022</td>
<td>N₂</td>
<td>2x10⁻⁵</td>
<td>5:77:18</td>
</tr>
<tr>
<td>5</td>
<td>0.050</td>
<td>N₂</td>
<td>4x10⁻⁵</td>
<td>55:34:11</td>
</tr>
<tr>
<td>6</td>
<td>0.073</td>
<td>N₂</td>
<td>-</td>
<td>69:26:5</td>
</tr>
<tr>
<td>7</td>
<td>0.065</td>
<td>N₂+H₂(1:1)</td>
<td>-</td>
<td>5:82:13</td>
</tr>
</tbody>
</table>

Table 5.1. List of grown samples. Sample 1 was grown at room temperature, all the others were grown at 350 °C.
5.3. Growth of mixed $\alpha$-Fe and $\gamma'$-Fe$_4$N samples

It is known that $\alpha$-Fe can be grown epitaxially on MgO(100) with its unit cell rotated 45° with respect to the substrate [4]. The misfit between the lattices of $\alpha$-Fe and MgO is 3.5%. We have demonstrated that Fe$_4$N grows epitaxially on this substrate as well [1, 2]. It grows without an in-plane rotation as it is often observed in complex oxides. The orientation relationship between the grown Fe$_4$N layer and the substrate is as follows:

$$[110]_\alpha \parallel [100]_{\text{MgO}}, (001)_\alpha \parallel (001)_{\text{MgO}},$$

$$[100]_{\gamma'} \parallel [100]_{\text{MgO}}, (001)_{\gamma'} \parallel (001)_{\text{MgO}}.$$  

The $\gamma'$-Fe$_4$N phase has a large mismatch with both $\alpha$-Fe and MgO (6.6% and 10.1% respectively). The $\alpha$-Fe phase has a body-centered cubic structure. The iron sublattice of the $\gamma'$-Fe$_4$N phase forms a face-centered cubic structure. These data make it surprising that the two phases can well coexist in a thin film, still being epitaxial according to the orientation relationships as will be shown next.

Sample 5 in table 5.1 consists of both $\alpha$-Fe and $\gamma'$-Fe$_4$N. The 2-axes pole XRD figures shown in figure 5.2 were taken at fixed scattering angles 20 corresponding to the reflections from (111) planes of $\gamma'$ and (110) planes of $\alpha$-Fe, respectively. The presence of four peaks

Figure 5.1. a) Mössbauer spectrum for sample 1 grown at room temperature. The fit (see text) is indicated by a full line; the fitted components are indicated by dashed lines. b) Mössbauer spectrum for sample 2 grown at 350°C. c) XRD spectra in specular geometry (upper) and with an offset of 6° (lower) of sample 1; d) XRD spectra in specular geometry (upper) and with an offset of 6° (lower) of sample 2.
indicates that the crystallites of both phases are oriented according to the orientation relationships for epitaxial growth given above. The iron peaks in the plot were a bit sharper than those of iron nitride, which indicates a slightly higher degree of mosaicity of iron nitride grains. The width of the peaks in the 0-20 scans were broadened due to the small thickness of crystallites and due to defects. The broadening due to defects of the (002) peak of \( \gamma' \) was quite small and almost the whole broadening can be ascribed to the size of the crystallites, which, in the direction perpendicular to the surface, we assume to be equal to the film thickness (250Å). The (002) reflection from iron was broader, which indicates a higher density of defects and/or a smaller (but not smaller than 150Å) grain size. These observations indicate that the layer consists of patches of the two phases with a thickness close to the thickness of the film. This conclusion is confirmed by AFM measurements to be described below.

The minimum yield observed in channeling experiments is defined as the ratio between the backscatter yield from the whole layer thickness, obtained with the beam oriented in a main crystalline direction and in a “random” direction. It is a good indicator for the crystalline quality of an epitaxially grown layer. For sample 5 we observed for Fe a minimum yield of 60% in the <001> crystalline direction. This implies that at least one of the grown phases was well epitaxial.

![XRD pole figures](image)

**Figure 5.2.** XRD pole figures measured for sample 5 at a fixed scattering angle 2\( \theta \) corresponding to the (110) reflection from \( \alpha\)-Fe, and the (111) reflection from \( \gamma'\)-Fe\(_4\)N, respectively.
An AFM scan of the surface of sample 2 consisting of both iron and iron nitride phases in about equal quantities is shown in figure 5.3. This sample exhibited properties similar to sample 5 concerning the XRD and had well oriented grains of both Fe₄N and Fe. The scan shows high and low patches elongated along the <100> direction of α-Fe, which is equivalent to the <110> direction of MgO. The difference in height between the high and low patches is ~6 nm. The height difference might have increased after oxidation in air. The width of the higher patches is ≥ 200 Å and their length can be as large as 1000 Å. We attribute higher and lower patches to grains of α-Fe and γ’-Fe₄N. Together with the XRD and channeling data this leads to a picture of growth, whereby crystallites of Fe and of Fe₄N grow separately, most probably forming a columnar structure. This implies that N atoms landing on an iron crystallite migrate to an adjacent Fe₄N crystallite over distances up to 200 Å, before being incorporated in the growing layer. As the sticking coefficient of N atoms was found to be unity, the loss of N atoms during diffusion due to recombination to N₂ molecules and subsequent desorption must be very small. Iron atoms must be also very mobile at this temperature. Because of this high mobility, combined with the low growth rates applied in the present work, it is probable that the growth proceeds mainly by step flow or by layer-by-layer. The elongation of the patches along the <110> surface direction of the MgO substrate might be explained by the prevailing direction of steps at the MgO surface, which is also <110>.

Figure 5.3. AFM scans of the mixed sample 2 taken in contact mode. The scan range was 1x1 µm², the total vertical gray scale corresponds to 8 nm. The higher features are elongated along the <110> direction of MgO.
A detailed experimental investigation of the diffusion process of N atoms on the surface of a single Fe(100) crystal was recently published by Pederson et. al. [5]. According to their results, at temperatures between 300 and 325 K N atoms can survive at an iron surface for a long time (at least tens of minutes) at low coverages of the order of 0.1 monolayer. The hopping rate of N atoms on this surface was measured at room temperature. Assuming an exponential dependence on temperature of the hopping rate of N atoms, this rate would be \( \sim 10^5 \text{s}^{-1} \) at a temperature of 350°C as used in our experiments. At this high mobility a trajectory of a randomly walking particle can be extremely long in the time needed to grow a small fraction of one atomic layer. During this walk the chance for recombination to N\(_2\) should be very low, which can be concluded from the high sticking probability. This is in accordance with another conclusion of Pederson et. al., namely that there is a strong repulsive nearest-neighbor interaction between two N atoms at the surface as a result of the high binding of a N adatom in fourfold coordinated positions of the Fe(100) surface and of a lattice-mediated effect. Their conclusion, that N atoms can cover a large distance over a surface of an Fe(100) crystallite without recombination, is in agreement with our findings.

Sample 6 in table 5.1, which was grown without hydrogen, consists of only 26% of \( \gamma' \) as was derived from CEMS. The intensity of the (002) peak of \( \gamma' \) in the \( \theta/2\theta \) XRD scan was too small to be observed, which indicated a different orientation of the \( \gamma' \) crystallites. Tilting of the sample off the specular geometry at a scattering angle fixed to the value corresponding to the (002) \( \gamma' \) peak revealed the distribution of the orientation of the crystallites. The highest intensity of the peak was found at 6.5° off the specular geometry. This value is too big to be explained by a substrate miscut. This misorientation can be related with nitriding experiments done earlier in our group [6]. The post-nitriding of epitaxial layers of iron in a mixture of NH\(_3\) and H\(_2\) was found to result in the formation of four structural domains of \( \gamma'\)-Fe\(_4\)N, which were tilted by 6.2° with respect to the [001] direction of the MgO substrate. This observation can be understood assuming a Bain type phase transition from the bcc to the fcc iron sublattice [7]. Using this information, our observation can be explained assuming a simple growth mode of \( \gamma'\)-Fe\(_4\)N layers in this case, where the growth occurs in two steps: first, the epitaxial growth of iron and, second, the nitriding of the \( \alpha\)-Fe(100) layer in the flux of atomic nitrogen. Obviously, this two-step growth mode is in competition with the growth mode where Fe\(_4\)N crystallites are grown from Fe plus N directly, leading to epitaxial \( \gamma' \) crystallites. In comparison with other samples, this sample was grown in the lowest flux of nitrogen with respect to the flux of Fe. Our finding that the two-step growth mode occurs only at low N fluxes is in agreement with this picture of competing growth modes, where the indirect mode is favored in the absence of sufficient Fe\(_4\)N crystallites with the proper orientation, which serve as nucleation sites.

### 5.4. Possible role of hydrogen

As was shown above, the admixture of hydrogen in the working gas of the RF-source increases the content of nitrogen in the film. It also promotes the formation of Fe\(_4\)N (see chapter 3). Hydrogen can affect the uptake of nitrogen in the sample in the following steps: 1) it can increase the efficiency of the source, 2) it can decrease the recombination rate of atoms into molecules at the walls of the Teflon tube, 3) it can also improve the uptake rate of nitrogen at the surface of the sample. In order to find out in which step hydrogen plays the most crucial role, we tried to exclude the influence of hydrogen on the efficiency of the RF-source and in the Teflon tube used for transport by using pure nitrogen as a working gas. This was done by applying a background pressure of \(~10^{-3}\) mbar H\(_2\) gas in the UHV chamber, so that it could be adsorbed
The channeling dips of Fe are shifted with respect to the ones for Mg by up to ~0.2° (see figure 5.4), as is the case in nearly all epitaxial layers we have grown so far [2]. Our layers have a very small tetragonal distortion as can be concluded from the angular position of the dips in channeling spectra. In case of a tetragonally distorted lattice of Fe₄N the <110> dips from Mg and from Fe would be at different positions corresponding to the angle between the [110] planes of tetragonal and cubic lattices. But the dips of Mg and Fe coincide quite perfectly in the ψ and φ scans. The shifts observed in the θ scans must be due to a tilt in a certain direction of the lattice of iron nitride with respect to the lattice of the substrate. Such a tilt can be caused by a preferential orientation of step edges at the surface of the substrate, due to a small miscut, combined with a lattice mismatch between the substrate and the grown layer. [12, 13]. No detailed model to explain this effect for our case is presented here. The result is that the scans, shown in figure 5.4, cannot be measured precisely through the true dip position simultaneously for Mg and Fe. This explains the variation in the relative minimum yields for Fe and Mg. The minimum yield for Fe in both the <100> and the <110> string directions was 11%, which is close to the calculated value of 8% for a scan along the [001] plane through the <100> axis of a perfect crystal. The calculation was done with a program-code developed by dr. V.A. Khodyrev.

Figure 5.5 shows “random” and channeling spectra along <100> and <110> directions. Channeling peaks of iron contain two maxima, one of which (the right one) is a surface peak and the second one is the interface peak. The surface peak arises because several topmost layers are not fully shadowed and a certain effective number of Fe planes parallel to the surface is “seen” by the ion beam. Atoms of deeper layers are better shadowed by surface atoms. The peak at the interface with the substrate arises probably because of a higher density of defects in this region of the layer. However, this peak is not very high and the sample is considered to be very close to a single-crystal.

![Figure 5.5](image.png)

**Figure 5.5.** Channeling in a sample grown on a cleaved MgO(100): a) “random” and channeling along <100> direction spectra; b) “random” and channeling along <110> direction spectra.
Mechanism of growth of Fe₄N on MgO(100)

at the surface of the sample. It is known that hydrogen adsorbs and dissociates at an iron surface [8].

The conditions of growth and the characteristics of the grown samples to compare are listed in table 1, samples 3-6. The substrate temperature was kept at 350°C. The growth rate was chosen such that in the case of pure nitrogen in the source and no background pressure of hydrogen in the chamber the sample would be nitrided incompletely, resulting in a mixture of α-Fe and γ'-Fe₄N. As can be seen from the results in the table, the uptake of nitrogen was about the same in all these cases. The presence of hydrogen has resulted in a small difference in the distribution of the phases but did not change the total uptake of nitrogen (compare sample 3 and 4, 5 and 6, which have about the same growth rate). According to the channeling experiments, the sample grown in hydrogen exhibits a better crystalline quality and clear channeling dips were observed.

The effect of hydrogen in the RF-source was demonstrated in the last sample in table 1 where a mixture of the two gases was used. The uptake of N has increased by a factor of 3 with respect to other samples while the partial pressure of N₂ in the RF-source was the same as used for the production of the other four samples.

Another observation we made is that the presence of hydrogen at the surface promotes the direct growth mode. This can be seen by comparing samples 5 and 6. The presence of hydrogen at the surface during growth of sample 5 in the low flux of nitrogen promoted the direct growth mechanism and an epitaxial γ’ layer was grown. In sample 6, grown in the absence of hydrogen and in the low flux of atomic N, the two-step growth mechanism dominated.

Another effect due to the presence of hydrogen was found in our earlier work. In the case of high N fluxes the ε-FeₓN phase with a higher nitrogen content is formed in the absence of hydrogen. We found that in case excess nitrogen is present, so that the ε phase could be formed, layers consisting of the pure γ’ phase are grown if hydrogen is present. This implies that the excess nitrogen can escape in the presence of hydrogen, possibly by the formation of NHₓ (x=1-3) complexes.

The fact that hydrogen does not change the uptake of nitrogen at the surface is not unexpected, since we know that the sticking coefficient of N atoms to iron surface is unity under all circumstances applied here. The increase of nitrogen uptake while using a mixture of gases in the RF-source can be only explained by a higher efficiency of the source plus the Teflon tube used for transport. This effect was observed before in atomic oxygen sources [9, 10] and was explained by a reduction of the recombination at the walls of the container due to the passivation of the walls by hydrogen. In order to reduce the recombination rate at the walls, the boiling in boric acid of the Pyrex container was implemented (see Chapter 4). The presence of hydrogen in a treated container did not have a big effect on the efficiency of the source. This is again in agreement with the work published on atomic sources of O [9, 10].
5.5. Channeling study of a sample grown on a cleaved MgO(100)

For the growth of all samples described so far a polished single-crystalline MgO(100) substrate was used. Polishing introduces defects at the surface, which mostly are removed by annealing. As an alternative to a polished substrate, a cleaved MgO slab can be used. A cleaved and annealed MgO surface consists of high steps and long terraces, but the crystal has a lower mosaicity and the terraces are atomically flat [11]. No extra defects are introduced in this case. A cleaved substrate was used to grow an Fe$_4$N layer under optimal conditions, using a mixture of hydrogen and nitrogen in the RF-source. The film was of particularly good quality and exhibited very good channeling in the <100> as well as in the <110> directions (figure 5.4). The channeling dips were measured in two perpendicular scan directions. For the scan through the <100> direction these directions were along the (010) and the (001) planes; for the <110> dip these directions were along the (010) and the (101) planes. The CEMS spectrum showed the presence of pure Fe$_4$N with a component due to oxidation in air.

**Figure 5.4.** Channeling scans for Mg and Fe in the best sample, grown on cleaved MgO(100) substrate.
5.6. Conclusions

In earlier work (see Chapter 3) we showed that it is possible to grow epitaxial layers of \(\gamma'-\text{Fe}_4\text{N}\) on a MgO(100) substrate in spite of the mismatch of \(\sim 10\%\) between their lattice parameters. It was found that the presence of hydrogen in the RF-source had a large influence on the uptake of nitrogen by the grown sample as well as on the crystalline properties of it. In this chapter the results of a study of the growth mechanism of \(\gamma'-\text{Fe}_4\text{N}\) on MgO(100) and of the influence of hydrogen are presented. We also demonstrated the possibility to grow a nearly perfect single-crystal of \(\gamma'-\text{Fe}_4\text{N}\). Most of the samples were grown so that two phases, namely \(\alpha\)-Fe and \(\gamma'-\text{Fe}_4\text{N}\), were present. The results of CEMS, XRD, RBS/channeling and AFM measurements on these mixed samples indicated that the layers have a columnar structure formed by crystallites of the two pure phases. The patches of \(\alpha\)-Fe and of \(\gamma'-\text{Fe}_4\text{N}\) are elongated along the main [110] step direction of the MgO substrate. Surprisingly, both iron and iron nitride crystallites were epitaxial. This implies a growth mechanism, which requires a high mobility of N atoms on the Fe(100) surface and of Fe atoms on the surface of \(\gamma'-\text{Fe}_4\text{N}\). From the fact that the uptake of nitrogen was not dependent on temperature we concluded that the sticking coefficient of N atoms to the surfaces of \(\alpha\)-Fe and \(\gamma'-\text{Fe}_4\text{N}\) is unity. The study of a sample consisting of only 26% of the \(\gamma'\) phase indicated the occurrence of a second growth mode, which appears at low fluxes of atomic nitrogen and in the absence of hydrogen at the surface during the growth. In this growth mode first an epitaxial Fe layer is grown, which is subsequently transformed into the \(\gamma'-\text{Fe}_4\text{N}\) phase. The crystallites of \(\gamma'-\text{Fe}_4\text{N}\) in this layer are tilted by approximately 6.5\(^\circ\) from the epitaxial direction. We have also shown that a nano-crystalline layer can be grown at room temperature. It was observed that in the presence of hydrogen the pure \(\gamma'-\text{Fe}_4\text{N}\) phase is formed even when there is an excess of atomic nitrogen during growth, sufficient for the formation of an \(\varepsilon\)-Fe\(_x\)N phase containing more nitrogen [2]. This phase is formed in the absence of hydrogen. The hydrogen creates an escape route for the excess nitrogen, possibly by the formation of NH\(_x\) (x=1-3) complexes.

These facts can be explained by the following tentative model for the growth of \(\alpha\)-Fe/\(\gamma'-\text{Fe}_4\text{N}\) at temperatures in the range of 300-400 °C. In this model we do not describe the initial phase of the growth directly on the MgO substrate. The arriving atoms of Fe and N have a high mobility. Nitrogen adatoms move until they arrive at a patch consisting of Fe\(_4\text{N}\). There they are incorporated in the growing layer, probably at a step edge or at the edge of a growing island. Equally, the Fe adatoms move until they arrive at a step edge. This model implies a step-flow or a layer-by-layer growth mode for Fe and Fe\(_4\text{N}\). In the layer-by-layer growth mode monolayer height islands of the growing phase are formed and grow until they coalesce. For \(\alpha\)-Fe the growth mode has been studied as a function of temperature by Stroscio et al. [14]. Their RHEED oscillations measured at a growth temperature of 250 °C could indicate a mixture of layer-by-layer growth and step flow growth. This observation makes it probable that at higher substrate temperatures step flow growth for \(\alpha\)-Fe is to be expected. If Fe adatoms arrive at a step edge where the lower layer consists of \(\gamma'-\text{Fe}_4\text{N}\), they will only be incorporated if a suitable surrounding, consisting of N and Fe adatoms, is encountered. In general, nucleation is an important factor in the growth. The presence of H atoms obviously facilitates the nucleation of \(\gamma'-\text{Fe}_4\text{N}\), possibly by changing the adatom mobility at the surface. This point is also illustrated by our observations that, at low N fluxes, the “one step growth” mode of Fe\(_4\text{N}\) is promoted by the presence of hydrogen.

The sample consisting of the pure \(\gamma'-\text{Fe}_4\text{N}\) phase with the best crystalline quality was grown on a cleaved MgO(100) substrate. The channeling yield in the <100> string direction amounted to 11%, which is close to the calculated value of 8%. The discrepancy between the...
experimental and calculated numbers could be explained by the presence of defects at the interface with the MgO substrate. The slight tilt between the crystal axes in the MgO substrate and the grown layer could not be explained in detail.

5.7. References
