A Structural Viewpoint of Magnetism in Fe and Co Based Superlattices

MATTS BJÖRCK
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Abstract

In order to understand the properties of thin film devices, knowledge of the material’s structure is essential. The work presented here combines magnetic and structural characterization of the systems studied to gain a deeper physical understanding. The magnetic properties have been studied with a combination of x-ray magnetic circular dichroism, SQUID magnetometry and magneto-optical Kerr effect. For the structural characterization, x-ray reflectivity and diffraction have been used, complemented by neutron diffraction and transmission electron microscopy.

One structural property that affects the magnetic moment in metal-on-metal superlattices is interdiffusion between the layers. This is discussed for bcc Fe/Co(001) and bcc Fe$_3$Ni$_7$/Co(001) superlattices. The effect of interdiffusion was seen as a large region of enhanced magnetic moments as compared to theoretical calculations, which assume perfectly sharp interfaces. For the Fe$_3$Ni$_7$/Co(001) superlattices the chemical interface region, as revealed by neutron diffraction, was in good agreement with the region of magnetic enhancement.

Another structural property that has been investigated is the strain in the magnetic layers. This does not affect the spin magnetic moment to a large extent. However the magnetocrystalline anisotropy and the orbital moment are affected by the presence of strain. The effects on the orbital moment from strain and interfaces for Fe in Fe/V superlattices was studied, and it was found that the two contributions were separable.

In this context the effect of strain on the out-of-plane magnetocrystalline anisotropy in FeCo/Pt has also been studied. The latter system is interesting from a technological perspective since tetragonally distorted FeCo alloys have the potential to be suitable new materials in computer hard drives.

Finally, a computer program, based on the Differential Evolution algorithm, to refine primarily x-ray reflectivity data, is presented.

Keywords: Magnetism, Multilayer, Superlattice, X-ray magnetic circular dichroism, X-ray diffraction, X-ray reflectivity, Neutron diffraction, Structural refinement, Interfaces

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Videnskaben!
- prof. Bondo
List of Papers

This thesis is based on the following papers, which are referred to in the text by their Roman numerals.

I  Element-specific magnetic moment profile in BCC Fe/Co superlattices
M. Björck, G. Andersson, B. Lindgren, R. Wäppling, V. Stanciu, P. Nordblad

II Depth selective investigations of magnetic multilayers by X-ray resonant magnetic reflectivity
M.A. Andreeva, A.G. Smekhova, B. Lindgren, M. Björck and G. Andersson

III Element-specific magnetic moments in bcc Fe_{81}Ni_{19}/Co superlattices
I.L. Soroka, M. Björck, R. Brucas, P. Korzhavyi, G. Andersson

IV The asymmetric interface roughness of Fe_{82}Ni_{18}/Co superlattices as revealed by neutron diffraction
M. Björck, I. L. Soroka, C. Chacon-Carillo, G. Andersson

V Perpendicular magnetocrystalline anisotropy in tetragonally distorted Fe-Co alloys

VI Structure of Fe-Co/Pt (001) superlattices: a realization of tetragonal Fe-Co alloys
G. Andersson, M. Björck, H. Lidbaum, B. Sanyal, C. Chacon, C. Zlotea, S. Valizadeh

VII Magnetic anisotropy of tetragonal FeCo/Pt (001) superlattices
P. Warnicke, G. Andersson, M. Björck, J. Ferré and P. Nordblad
VIII  Magnetic moments in FeCo/Pt (001) superlattices
M. Björck, G. Andersson
In Manuscript.

IX  The effects of strain and interfaces on the orbital moment in Fe/V superlattices
M. Björck, M. Pärnaste, M. Marcellini, G. Andersson, B. Hjörvarsson

X  GenX: An extensible X-ray reflectivity refinement software utilizing Differential Evolution
M. Björck, G. Andersson
In Manuscript.

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Publications not included

The following publications are not included in this dissertation as they are not relevant to the present subject.

Stability of the induced magnetic V moment in Fe/V superlattices upon Hydrogen loading
A. Remhof, G. Nowak, A. Nefedov, H. Zabel, M. Björck, M. Pärnaste and B. Hjörvarsson

Remote control of the exchange splitting in magnetic heterostructures
A. Remhof, G. Nowak, H. Zabel, M. Björck, M. Pärnaste, B. Hjörvarsson and V. Uzdin
Comments on my participation

The level of my participation in the presented papers is somewhat reflected by my position in the author list. The following is a brief statement of the level of my involvement in the different papers.

<table>
<thead>
<tr>
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<tbody>
<tr>
<td>I</td>
<td>Grew and characterized the samples. Was responsible for the XMCD measurements and the data analysis.</td>
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<tr>
<td>II</td>
<td>Grew and characterized the sample. Participated in the measurements and tested the program written by M. Andreeva.</td>
</tr>
<tr>
<td>III</td>
<td>Responsible for the XMCD data analysis and interpretation.</td>
</tr>
<tr>
<td>IV</td>
<td>Conducted the neutron measurements and analyzed the data.</td>
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<tr>
<td>V</td>
<td>Participated in the experimental planning and conducted low temperature and high field MOKE measurements.</td>
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<td>VI</td>
<td>Same as V. Also, responsible for x-ray simulations and involved in the interpretation of the data.</td>
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<tr>
<td>VII</td>
<td>Same as V. In addition, took active part in the analysis and modeling of the data.</td>
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<tr>
<td>VIII</td>
<td>Grew and characterized the samples. Was responsible for the XMCD measurements and the data analysis.</td>
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<tr>
<td>IX</td>
<td>Grew some of the samples. Responsible for the XMCD measurements and data analysis. Took active part in the structural characterization.</td>
</tr>
<tr>
<td>X</td>
<td>Wrote and tested the program.</td>
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1. Introduction

During the last few decades the research on magnetism has shifted its focus from bulk materials to surfaces and interfaces, where the symmetry with respect to the bulk is reduced and new phenomena arise. The materials studied are in the form of thin films or particles/dots depending on the number of dimensions that are reduced. Such research was a natural step forward when the necessary technology for manipulating and building materials at an atomic scale had been developed. This knowledge is also actively sought by industry since manipulating materials at this level can produce better functionality as well as reduce the dimensions of the products. Perhaps the most striking example is hard disk drives for computers, the storage capacity of which has increased markedly with the aid of magnetism research. For example, the research on the giant magnetoresistance (GMR) effect and spin dependent tunneling directly produced a marked increase in the storage capacity of hard drives. At present there is an active search after better materials for the recording media in the hard drives. In the future the spin degree of freedom might even be incorporated into the electronic circuits with the aid of a spin transistor. All this progress relies on a firm understanding of the magnetic properties of materials on the atomic scale.

The work presented in this dissertation concerns the magnetic properties of interfaces and thin films. A convenient way to study interfaces is to produce multilayers where the structure to be studied is repeated a number of times. In this way a large amount of material with interface properties can be produced which makes it possible to study interfaces with probes otherwise used for bulk materials. In order to measure the intrinsic properties of the multilayer it is desirable to have them in the form of single crystals. This makes the crystallographic orientations well defined while removing the largest defects, namely grain boundaries. A picture of an ideal superlattice, a single crystalline multilayer, can be seen in figure 1.1. The figure shows the multilayer structure in the background and an enlarged region showing the crystalline order between the different constituents of the superlattice. However, it is close to impossible to grow a superlattice as the one shown in figure 1.1. The nature of the growth process will produce roughness. Thus, the interfaces between the materials will not be completely flat. In addition, the different constituents can have a tendency to mix with each other and form alloys at the interfaces. Finally, crystalline defects such as dislocations can occur during growth. Also, relaxation of the strained layers can occur if the system is not lattice matched, i.e.
the layers have different bulk lattice constants. In order to understand the magnetic properties it is required to have a firm understanding of the structure of the samples. Therefore this dissertation is not devoted only to the magnetism of superlattices but also to some extent to the structure.

The dissertation is based on the work presented in the papers. The purpose of this introduction is to give the reader a brief background to the publications that are included. First the growth technique and defects arising in the produced structures are presented in chapter 2. Next, chapter 3 presents the various magnetic phenomena studied (magnetic moments and anisotropy) with emphasis on thin film systems. The background for structural characterization is discussed in chapter 4, especially for the case of superlattices and multilayers. Chapter 5 presents the techniques used for characterization of the magnetic properties. The latter section focuses mainly on x-ray magnetic circular dichroism which has been one of the major methods used. However, the chapter also deals with the magneto-optical Kerr effect and magnetic neutron scattering. Finally, a summary of the papers included in the thesis is provided in chapter 6.
2. Layer Growth

The superlattices presented in this work have been grown by a technique called magnetron sputtering. A brief introduction to the physical process of sputtering will be given in this chapter. The sputtering source creates a flux of atoms that will condense onto a substrate. In order to achieve the growth of a single crystal it is usually necessary to have a single crystal substrate. When the atoms land on the surface they can adapt themselves to the crystal structure of the substrate. If the grown film and substrate have a relation between their crystallographic directions the growth is denoted as epitaxial.

Defects can significantly affect the physical properties of the materials. These defects range from ordinary defects in crystals, such as dislocations and grain boundaries, to defects more inherent to thin film growth. These include interdiffusion, i.e. the constituents mix, and roughness of the interfaces. The second section is thus devoted to a review of the different phenomena and defects arising during thin film growth.

2.1 Sputtering

This section focuses on the physical picture of the sputtering process and especially the branch called magnetron sputtering. For details of the systems used the reader is referred to earlier dissertations [1, 2]. The explanation given in this section is a condensed version of the vast literature on the subject of sputtering given in [3].

The corner stones for sputtering are the materials to be deposited, targets, and the sputter gas, usually a noble gas like Ar. To create a material flux from a target a plasma is created in front of the target. In the simplest configuration the sputter gas is introduced into the chamber and a negative voltage is applied to the target. When the voltage is high enough, at the breakdown voltage, it will start to ionize the gas and accelerate the ions toward the target. Upon increasing the voltage the plasma will become self-sustained when each incident ion produces enough electrons to produce one more ion. A dc glow discharge usually needs a pressure of 20–100 mtorr, 3–13 Pa.

The purpose of magnetron sputtering is to make more efficient use of the secondary electrons emitted from the target. This can be achieved by applying a magnetic field parallel to the surface of the target. The electrons will be confined closer to the surface and hence locally increase the ionization rate. A typical configuration can be seen in figure 2.1. The increased ionization
rate will cause a higher deposition rate but can also be used to decrease the pressure of the sputtering gas, usually by an order of magnitude.

Some of the work in this thesis is devoted to the study of alloys as a constituent of the multilayer. To deposit an alloy by magnetron sputtering there are in general two possibilities. The first is to make an alloy target with the desired composition. The flux of atoms from such a target will have the same composition as the target provided that the target has been sputtered long enough. This is due to a self-regulating process: if one of the constituents has higher sputtering yield than the other the surface will be enriched with the other material until a steady state has been reached. The second way to deposit an alloy is to cosputter the constituents from two separate magnetrons. Usually an alloy target is simpler to use than cosputtering since the composition is fixed. However, if the composition is to be varied cosputtering is the preferred way. Cosputtering was used to fabricate the (Fe,Co)/Pt superlattices presented in papers V–VIII while an alloy target was used for the fabrication of the Fe$_{0.82}$Ni$_{0.18}$/Co superlattices, see papers III and IV.

To reduce the contaminants in the deposited material, sputtering requires a high purity gas. The Argon gas used for the samples grown in these studies has a purity of 99.9999\% which roughly corresponds to a background pressure of $10^{-9}$ torr. Together with rather high deposition rates, 0.05 nm s$^{-1}$, this results in final high purity materials of at least 99.8\%. It should be noted that the as-supplied purity of the materials is above 99.9\%.

### 2.2 Film Growth

Epitaxial growth can be used to achieve materials with crystal structures far from the bulk structures found in nature. Examples of this include the stabi-
lization of bcc Co which has a hcp structure in the bulk [4]. The growth of bcc Co can be promoted by an underlying Fe layer which has a bcc structure and provides the stabilization of bcc Co up to about 8 atomic layers [5]. After this the Co layer starts to transform to the fcc structure. If the constituents of the superlattice have lattice parameters that are far from each other the material grown will be under considerable strain. The strain that can be induced in thin films can become quite sizable, with distortion of the lattice parameters of several percent. This effect was used to fabricate bcc FeCo alloys with \( c/a \) ratios quite different from the bulk, around 1.2 compared to 1. These large distortions can give different physical properties of the materials, for example large changes in the magnetocrystalline anisotropy as compared to the bulk [6, 7].

There will be a critical thickness where the layer starts to relax through misfit dislocation and finally regains its bulk structure. The thickness where the layer starts to relax is usually denoted as the critical thickness of the layer. This type of relaxation can occur for the superlattice relative to the substrate, paper I, as well as between the constituents of the superlattice.

Classically three different growth modes of a crystal are discussed [8], each of them named after their investigators:

- Frank-Van der Merwe (FV) growth, which is perfect layer-by-layer growth where one atomic layer is deposited after the previous atomic layer is completed.
- Volmer-Weber growth (VW) growth, which is three dimensional growth where the film nucleates directly onto the substrate and forms isolated crystallites
- Stranski-Krastanov (SK) growth, which is initial layer-by-layer growth followed by a transition to three dimensional growth. This is an intermediate mode between the previous two.

The growth mode of a layer is determined by the the surface energies of the underlaying layer, the deposited layer and the interface [8]. However, also dynamical processes affects the growth mode such as diffusion length of the atoms on the surface. In addition, deposition by sputtering involves high energy particles impinging on the surface, which can also modify the behavior.

The sections below will deal with the parametrization of the various defects that can arise in thin films and especially multilayer structures. These concepts are used in chapter 4 and throughout the papers.

### 2.2.1 Crystalline Defects

Real crystals possess a kind of crystal imperfection known as mosaic structure [9], which is schematically shown in figure 2.2. This structure consists of grains of perfect crystals that are slightly rotated with respect to each other. The regions of perfect crystals are thus separated by dislocations. To parameterize the degree of perfection of a thin film the concepts of in-plane and
out-of-plane correlation lengths are introduced. The correlation length in one direction is the mean size of perfect crystal blocks along that direction. The term mosaicity is the angular spread of the misorientation of the crystal blocks relative to each other. The defects forming these features can originate from relaxation of the film relative to the substrate, as described above. Alternatively, the defects can originate from the interfaces between the constituents or the growth process itself. In addition, defects in the substrate can propagate through the film.

2.2.2 Layer Imperfections

Even for FV growth there will be some roughness associated with film growth since the atoms will have a finite diffusion length. Thus, all interfaces will show some kind of roughness. Also, the roughness from the underlaying layers can be replicated through the film. If successive interfaces possess the same shape of interface profiles, they are said to be completely correlated, see figure 2.3. The other extreme case of roughness is completely uncorrelated roughness where there is no replication between the interfaces. As can be seen in figure 2.3 films with correlated will have no thickness fluctuations. On the other hand, films with uncorrelated roughness will have thickness fluctuations. In real films roughness is never completely correlated or uncorrelated which will be discussed further in section 4.3.1.
Another defect that can arise between different layers is interdiffusion of the materials. In contrast to roughness, which locally gives a chemically sharp interface, interdiffusion will result in a diffuse interface. One way to estimate if two materials has a tendency to intermix is to study the, usually readily available, bulk phase diagram. However, these phase diagrams is made for the bulk alloys and thus not necessarily applicable to thin films. Another way is to study the surface segregation energies for the different growth scenarios. This gives an indication whether or not it is energetically favorable to form a surface alloy. A compilation of surface segregation energies for a wide range of metallic materials can be found in [10, 11]
3. Thin Film Magnetism

This chapter deals with the background of the magnetic phenomena studied in this dissertation. First, the origin of ferromagnetism in 3d metals is presented with the Stoner model [12]. This explains why some metals develop ferromagnetism. The Stoner model deals with the spin moment of the electron. Although this is the major contribution in 3d metals there exists another contribution, the orbital moment. This moment arises due to the orbital motion of the electrons. Next, the dependence of the size of the magnetic moment in alloys and thin films on composition and interfaces is reviewed.

Another magnetic phenomenon discussed in the papers is the magnetocrystalline anisotropy which is the subject of the rest of the chapter. This phenomenon manifests itself by aligning the magnetic moment in preferential directions relative to the crystal structure. The different energy contributions to the magnetocrystalline anisotropy are reviewed. In addition, the connection between the orbital moment and the magnetocrystalline anisotropy is briefly discussed.

3.1 Itinerant Ferromagnetism

In 3d atoms magnetism arises from the 3d levels which are partly filled according to Hund’s rules and thereby form a net magnetic moment. In the case of metals the orbitals will overlap and form bands. For 3d metals the high lying 3d electrons will become delocalized, itinerant. Perhaps the simplest model that predicts ferromagnetism in metals is the Stoner theory. In the next paragraphs the Stoner criterion for ferromagnetism will be reviewed.

Let us make the assumption that the paramagnetic density of states (DOS) is known and does not depend on the band filling. Thus the energy of the electrons in the band is

$$E_B = \int_{E_\uparrow}^{E_\downarrow} E D_S(E) dE + \int_{E_\uparrow}^{E_\downarrow} E D_S(E) dE$$

(3.1)

where $E_\uparrow$ and $E_\downarrow$ are the Fermi energies of the spin up and down bands, respectively. $D_S(E)$ is the paramagnetic DOS per spin. In order to express the energy in more usable quantities, the DOS can be related to the total number of electrons in the $d$ band, $N$, and the spin polarization, $s$, as

$$\int_{0}^{E_\uparrow} D_S(E) dE + \int_{0}^{E_\downarrow} D_S(E) dE = N$$

(3.2)
By assuming a small spin polarization, replacing $D_S(E)$ by $D_S(E_F)$, and subtracting a zero point energy term the electron energy can be expressed as

$$E_B = \frac{N^2}{4D_S(E_F)} s^2$$  \hspace{1cm} (3.4)

Following Stoner [12] the exchange interaction can be expressed by the energy term

$$E_{ex} = -\frac{I}{4} (N_\uparrow - N_\downarrow)^2 = -\frac{I}{4} s^2 N^2$$  \hspace{1cm} (3.5)

where $I$ is the Stoner exchange parameter. The above equation contains a contribution from the Coulomb repulsion that arises from the fact that two electrons with the same spin cannot occupy the same local orbital, cf. Pauli’s exclusion principle for atoms. In addition it contains the magnetic exchange between the electrons.

Adding equation (3.4) and (3.5) gives the energy

$$E_B = \frac{N^2}{4} \left( \frac{1}{D_S(E_F)} - I \right) s^2$$  \hspace{1cm} (3.6)

To obtain a spontaneous spin polarization the factor inside the parenthesis has to be negative, that is

$$D_S(E_F) \geq 1/I$$  \hspace{1cm} (3.7)

This equation is the Stoner criterion for ferromagnetism. In figure 3.1 it can be seen that the only elements that satisfy the Stoner criterion are Fe, Co and Ni. The values in the graph are taken from [13, 14].

The reason for magnetism in the metals at the end of the 3$d$ series is mainly the large density of states at the Fermi level. The Stoner exchange parameter is clearly of secondary importance as can be seen in figure 3.1. The reasons for the large density for the late 3$d$ metals are several: first of all the 3$d$ band must accommodate 10 electrons, and secondly the $d$ band is contracted with increasing atomic number due to the increasing nuclear charge. In fact, given the above discussion, it would be intuitive to believe that also elements such as Rh and Pd should be ferromagnetic. But since the 4$d$ electrons are further from the core they also extend further out. Consequently the bands broaden and have a lower density of states at the Fermi level. Hence, the only pure transition metals that exhibit ferromagnetism are the late 3$d$ metals.

### 3.2 Magnetic Moments

Although the Stoner criterion correctly predicts the existence of itinerant ferromagnetism it does not give the atomic magnetic moments. To explain the
The Stoner criterion for some metals. The full circles show the density of states at the Fermi level. The open circles display $1/f$ which is the border between ferromagnetic and paramagnetic elements.

<table>
<thead>
<tr>
<th>Element</th>
<th>$n$</th>
<th>$m$ [$\mu_B$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe</td>
<td>8</td>
<td>2.23</td>
</tr>
<tr>
<td>Co</td>
<td>9</td>
<td>1.73</td>
</tr>
<tr>
<td>Ni</td>
<td>10</td>
<td>0.62</td>
</tr>
</tbody>
</table>

Table 3.1: The number of valence electrons, $n$, and the atomic magnetic moment, $m$, for the ferromagnetic 3d metals [13].

measured magnetic moments for the 3d metals in a simple way, the important concept of strong and weak ferromagnetism has to be introduced. Cobalt and nickel are examples of strong ferromagnets, where the spin up band is completely filled with 5 electrons. Iron on the other hand is an example of a weak ferromagnet, where the spin up band is only partially filled.

Since a strong ferromagnet has the spin up band completely filled, its magnetic moment can be estimated from the number of valence electrons in the atom [13, 15]. As the spin up band is completely filled and contains 5 electrons, and the element has $n$ valence electrons in total (the number of 3d and 4s electrons) the atomic magnet moment, $m$, in bohr magnetons can be calculated as

$$m = 5 - (n - x - 5) = 10 - n + x$$

(3.8)

where $x$ is the number of 4s electrons per atom. In isolated atoms of Fe, Co and Ni the number of 4s electrons is 2 but in a metallic crystal the 4s electrons will spill over to the 3d band. In order to reproduce the measured magnetic
moment the 4s band must contain only about 0.65 electrons [13]. This will lead to moments of 1.65 \( \mu_B \) and 0.65 \( \mu_B \) for Co and Ni, respectively, which is in rather good agreement with the values reported in table 3.1. The same calculations for Fe would yield a moment of 2.65 \( \mu_B \) which is clearly too high. This value is actually the case for Fe as a strong ferromagnet. The "d-count" approach can also be used to explain alloys between different 3d elements, which exhibit strong ferromagnetism. Then the alloying is taken as a change in the mean number of electrons for a compound. This simple model explains the descending branch of the Slater-Pauling curve [13, 15], which displays the magnetic moment as a function of the number of 3d+4s electrons.

Since the main emphasis in this thesis has been on element specific studies of various 3d metal multilayers it is appropriate to explain why there exist atomic moments in materials that until now have been described as having delocalized electrons. In the above treatment, alloys are treated as a mix of elements, which only gives a total average moment. In reality the 3d bands are sufficiently localized to be said to belong to one type of atoms. Although the electrons can travel from atom to atom, each atomic species in an alloy can be considered to have its own magnetic moment. This has been shown for a variety of metals with for example neutron scattering [16]. For a further discussion of this subject see [15].

3.2.1 Thin Films

In this section some ideas on how and why the magnetic moment changes at interfaces will be presented. This is a vast area of research and a large number of materials combinations have been studied both as multilayers and as bilayer films [17–23]. It should be said that how and why the magnetic moments change is not only relevant to basic research, but also to applied research, as they influence e.g. the giant magnetoresistance effect and the properties of spin polarized tunneling, which are used in the reading heads of today’s hard drives.

A surprisingly good model of magnetic interfaces is the so-called local concentration model [24]. Although mostly used in computational physics, it provides an excellent intuitive tool for predicting how the spin moment changes at interfaces. The core of this model is to assume that the atoms are "near-sighted" regarding their chemical environment. This approximation leads to that the moment for a certain interface is calculated from the concentration in each layer. For a perfect bcc (001) interface the layer concentration at the interface is 1, although the local concentration will be 0.5 since each interface atom has 4 nearest neighbors of each element that take part in forming the interface. This model has also been extended to rough and interdiffused interfaces [25, 26]. If Fe/Co superlattices are compared to the alloy counterpart [16] it is easily seen that the magnetic moment for Fe should be enhanced to about 2.9 \( \mu_B \), whereas the Co moment should remain constant at about 1.8 \( \mu_B \).
This is in rather close agreement with the findings in paper I, where a Fe moment of 3.0 µB was found at the interface and the Co moment was constant at 1.6 µB.

The second contribution to the magnetic moment, the orbital moment, is not as easy to make simple quantitative estimates about. At interfaces the crystal field will change due to the change in the atomic environment. For 3d metals this usually leads to an unquenching of the orbital moment, and this effect can be large at the vacuum/metal interface [27]. Van der Laan [28] compiled some suggestions for why the orbital moment should increase at interfaces/surfaces and most of them fall into the category above, namely symmetry breaking and unquenching. However, also band filling can affect the orbital moment due to the change in orbital occupation as new orbitals will be filled. Strain will also affect the orbital moment, as the symmetry will change. The effect on the orbital moment from strain and interfaces was studied in paper IX.

3.3 Anisotropy

The magnetic anisotropy manifests itself by aligning the magnetic moments in preferential directions. These directions are intrinsically coupled to the symmetry of the crystal lattice of the material.

From a phenomenological perspective the anisotropy energy can be expressed as a sum of different energy contributions. The contributions that are relevant to the phenomena studied in this thesis will be dwelt upon in the following. First, a magnetic field will cause a torque on the magnetic moments in the sample. The energy contribution for this can be written as

\[
\frac{E_H}{V} = -\mu_0 M_s H \cos(\Theta)
\]

where \(\mu_0\) is the permeability of vacuum, \(M_s\) the saturation magnetization, \(H\) the applied field and \(\Theta\) is the angle between the magnetization and the applied field.

3.3.1 Magnetocrystalline Anisotropy

The magnetocrystalline anisotropy is an intrinsic property of magnetic materials. The angular dependence of the magnetocrystalline anisotropy energy relates to the symmetry of the crystal itself. Thus, the magnetocrystalline energy can be expanded in a power series of direction cosines which satisfies the crystal symmetry. For a tetragonal crystal, ignoring higher order direction cosines, the expression for the anisotropy energy can be written as

\[
\frac{E_a}{V} = K_1 \sin^2(\theta) + K_2 \sin^4(\theta)
\]

where \(K_1, K_2\) are anisotropy constants and \(\theta\) is the angle between the \(c\)-axis, i.e. the major axis, and the magnetic moment. On the other hand for the more
symmetric cubic structure the lowest order direction cosines is of the fourth order. Thus, for a cubic crystal the anisotropy is usually expressed as

$$
\frac{E_a}{V} = K_1 (\alpha_1^2 \alpha_2^2 + \alpha_2^2 \alpha_3^2 + \alpha_3^2 \alpha_1^2) + K_2 \alpha_1^2 \alpha_2^2 \alpha_3^2
$$

(3.11)

where $\alpha_1 = \cos(\theta)$, $\alpha_2 = \sin(\theta) \cos(\phi)$ and $\alpha_3 = \sin(\theta) \sin(\phi)$ are the directions projected onto each of the crystallographic axes.

The magnetocrystalline anisotropy is thus strongly dependent on the crystal symmetry. The microscopic explanation is that the neighboring atoms in a crystal will exert an electric field, the crystal field, on the orbiting electrons. This will force the orbits to align themselves with the crystal field. As is known from basic quantum mechanics, an orbiting electron will have an orbital momentum which is coupled to the spin moment through the spin-orbit coupling. This means that the spin direction of the electrons will be influenced by the orbital moment which, as stated above, will be affected by the crystal field. Consequently, the symmetry of the magnetocrystalline anisotropy energy will be reflected in the anisotropy of the orbital moment. In the 3d series the spin-orbit coupling is rather weak as compared to the crystal field contribution. This will not only reduce the magnetocrystalline anisotropy energy, but it is also responsible for quenching the orbital moment. Since the crystal field is a static field the orbitals will try to adapt to the field and this is realized by forming standing waves. If, on the other hand, the spin-orbit coupling would dominate the orbital motion would be more like running waves, and the orbital moment would be unquenched, as is the case for 4f metals with their large spin-orbit coupling. An artistic view of the phenomena can be seen in figure 3.2.

### 3.3.2 Magnetoelastic Anisotropy

By subjecting a ferromagnet to strain the symmetry of the crystal changes and thereby also the magnetocrystalline anisotropy. This phenomenon is known

![Figure 3.2](attachment:figure3_2.png)

*Figure 3.2: Quenched (a) orbital motion, standing waves, created by four negative point charges. (b) shows an unquenched orbital motion, running wave. The crystal field favors (a) whereas the spin-orbit interaction favors (b).*
as magnetoelastic anisotropy. The inverse effect is magnetostriction where the dimensions of the sample change upon a change in the magnetization direction. The anisotropy energy per volume associated with the magnetoelastic effect can be written as [29]

\[
\frac{E_{me}}{V} = -K_{me} \cos^2(\phi)
\]  

(3.12)

where \( \phi \) is the angle between the magnetization and the plane of isotropic stress and

\[
K_{me} = -\frac{3}{2} \lambda \sigma = -\frac{3}{2} \lambda E \varepsilon
\]  

(3.13)

Here \( \lambda \) is the magnetostriction coefficient and \( \sigma \) is the stress which relates to the strain, \( \varepsilon \), through the elastic modulus, \( E \). In thin films grown on substrates, or as superlattice structures, strain is usually present due to the lattice mismatch between the constituents. The magnetoelastic contribution has the same symmetry as a tetragonal crystal and thus the two contributions are linked. For example, a cubic material as Fe or FeCo alloy can be distorted by strain to form a tetragonal structure.

This effect can be used to modify the materials properties as proposed for the FeCo/Pt system in [6, 7] and studied in paper V and VII. It should be noted that a linear relationship between the strain and the magnetoelastic contribution is only valid for moderate strains as shown in several papers [6, 7, 30].

### 3.3.3 Interface Effects

When a material is placed in contact with another in a heterostructure the physical properties of the first atomic layers will change. As described in the previous sections the magnetic moment will be affected by neighboring atoms. In the same manner the anisotropy can change at the interfaces. To model this it is customary to include an interface term [29]

\[
K = K_{V,b} + 2\Delta K_{int}/t
\]  

(3.14)

where \( t \) is the thickness of the magnetic material, \( K_{V,b} \) is the bulk volume contribution to the anisotropy energy and \( \Delta K_{int} \) is the change of the anisotropy constant at the interfaces. However, when applying this model care must be taken since the \( K_{V,b} \) term, at least, will contain a magnetoelastic contribution from the strain [29]. Since the magnetoelastic contribution depends on the strain, which in turn will show a thickness dependence, this must be taken into consideration. For a superlattice structure the strain and the thickness can be controlled individually and the different contributions can to some extent be resolved, see paper VII.
3.3.4 Shape Anisotropy and Domains

In contrast to the microscopic origins of magnetic anisotropy there is also an energy contribution from the stray field emanating outside the ferromagnetic material. This energy contribution is denoted shape anisotropy. It originates from the magnetostatic energy and is dependent on the spatial dimensions of the material. This contribution can be written as

$$\frac{E_d}{V} = \frac{\mu_0}{2} \vec{M}_s \vec{N} \vec{M}_s$$  \hspace{1cm} (3.15)

where $N$ is the demagnetization tensor. For a thin plate which is infinite in the plane $N$ is given by

$$N = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$  \hspace{1cm} (3.16)

These equations are only valid for a homogeneously magnetized body. Real macroscopic ferromagnets usually break up into domains to minimize the magnetostatic energy, making the above expression for the demagnetizing energy invalid. Figure 3.3 shows an artistic view of the minimization of the magnetostatic energy. For thin films the magnetostatic energy is especially important for materials with an out-of-plane easy axis of magnetization, since the magnetostatic energy will favor an in-plane direction. Therefore a so-called stripe domain formation can occur as seen in paper VII.
4. Structural Characterization

The most widely used tool for structural characterization in materials science is x-ray diffraction. In addition, the use of other particles, such as neutrons and electrons, provide complementary information to x-ray diffraction. They all give information about crystalline quality, stress, texture, composition and interface roughness. For layered structures, x-ray reflectivity probes the layered structure regardless of its atomic arrangements. Thus it allows probing of the composition, density and interface quality. In order to extract these parameters various models have to be fitted to the measured data. The basic theory of the diffraction and reflectivity techniques will be briefly reviewed here. Some models using these theories have been implemented into a fitting program called GenX. This program uses the differential evolution algorithm [31, 32] to fit a model to the data and is presented in the appendix and paper X.

4.1 Reciprocal Space

Diffraction is the most common way to determine the microscopic structure of a material. In this section the theory of a weakly scattering crystal, called the kinematic approximation, will be reviewed. The kinematic approximation ignores multiple scattering effects, refraction and absorption, thus greatly simplifying the calculation of the diffracted intensities. This theory is usually sufficient for diffraction of metallic multilayers although it will fail at small incidence angles as will be discussed in the next section. It will also fail for close-to-perfect crystals. In those cases the dynamical theory has to be applied [33].

The scattering amplitude from a solid in the kinematic approximation can be written as [34]

\[ F(\vec{Q}) = \int_V f(\vec{r}) e^{i\vec{Q} \cdot \vec{r}} d^3\vec{r} \]  

(4.1)

where \( \vec{Q} \) is the wave vector transfer, defined as the change in wave vector of the scattered wave as seen in figure 4.1, \( \vec{Q} = \vec{k}_{\text{out}} - \vec{k}_{\text{in}} \). The exponential term is the phase factor and \( f(\vec{r}) \) is the scattering length density.

For a crystalline solid the scattering amplitude can be written as a product of two factors, one originating from the unit cell, UC, of the material, and the
other from the lattice sum:

\[ F(\mathbf{Q}) = \int_{V_{UC}} f(\mathbf{r}) e^{i \mathbf{Q} \cdot \mathbf{r}} d^3 \mathbf{r} \sum_{\mathbf{R}_n} e^{i \mathbf{Q} \cdot \mathbf{R}_n} \] (4.2)

where \( \mathbf{R}_n \) is the position of the \( n \)'th unit cell. The integration of the unit cell can be exchanged to a sum over all the atoms in the unit cell by exchanging the scattering length density \( f(\mathbf{r}) \) to the scattering length for atom \( j \), \( f_j(\mathbf{r}) \).

\[ F(\mathbf{Q}) = \sum_{j} f_j(\mathbf{r}) e^{i \mathbf{Q} \cdot \mathbf{r}} \sum_{\mathbf{R}_n} e^{i \mathbf{Q} \cdot \mathbf{R}_n} \] (4.3)

where \( \mathbf{r}_j \) is the position of the \( j \)'th atom in the unit cell.

The positions where a Bragg reflection can occur are given by

\[ \mathbf{Q} \cdot \mathbf{R}_n = 2\pi \times \text{integer} \] (4.4)

The set of \( \mathbf{Q} \) vectors that fulfill this criterion defines the reciprocal lattice, \( \mathbf{G} \), of \( \mathbf{R}_n \):

\[ \mathbf{G} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* \] (4.5)

where \( \mathbf{a}^* \), \( \mathbf{b}^* \) and \( \mathbf{c}^* \) are the basis vectors of the reciprocal lattice and \( h \), \( k \) and \( l \) are integers. Thus, the condition for locating a reciprocal lattice point is

\[ \mathbf{Q} = \mathbf{G} \] (4.6)

This is known as the Laue condition. It should be noted that the contents of the unit cell will modulate the intensities of the Bragg peaks and this will depend on the type of atoms and their arrangement in the unit cell.

### 4.2 Diffraction from a Superlattice

In the following the diffraction from a superlattice structure will be reviewed. This will be done in the weak scattering limit using the kinematical approximation as presented in the previous section.

For a superlattice composed of two layers \( A \) and \( B \) the unit cell will consist of one repetition of \( A \) and \( B \). If \( \mathbf{Q} \) is restricted to be normal to the film
Figure 4.2: A figure showing a superlattice diffraction pattern for an ideal Fe/Pt superlattice with different lattice spacings of the Fe layer. The upper graphs show the diffraction pattern, full line, with the envelope function, dashed line. The lower graphs show the layer form factors for Fe, full line, and Pt, dashed line, with the out-of-plane lattice spacing given by the labels.

plane, \( \vec{Q} = Q_z \hat{z} \), the atomic scattering length can be exchanged to the in-plane averaged scattering length, \( f_A \) and \( f_B \), for each material. This leads to a one dimensional (1D) model of the superlattice. The diffracted intensity, \( I(Q_z) = |F(Q_z)|^2 \) can then be written as \[ I(Q_z) = L_N(A)^2 \left\{ |f_A|^2 L_{n_A}(d_A)^2 + |f_B|^2 L_{n_B}(d_B)^2 + 2|f_B||f_A|L_{n_B}(d_B)L_{n_A}(d_A) \cos(Q_z \Lambda / 2) \right\} \] (4.7)

where

\[ L_n(x) = \frac{\sin(Q_z nx/2)}{\sin(Q_z x/2)} \] (4.8)

The factor \( L_N(A)^2 \) describes the superlattice lines which have maxima for \( Q_z = \frac{2\pi}{\Lambda} m \) where \( m \) is an integer. These superlattice lines are modulated with the scattering from the individual layers, the first two terms in the curly brackets, and one term representing the interference from the individual layers. Thus, if the difference in lattice spacing between material \( A \) and \( B \) is large the diffraction pattern will consist of two separate maxima modulated by the superlattice lines. The different maxima of the modulated term will give the individual lattice spacings of the materials. On the other hand, if the difference in lattice spacing is small the two peaks will overlap and the interference term will give a large contribution. This can give a single broad maximum which
is modulated by superlattice lines. An example shown in figure 4.2 where the simulated pattern from a Fe/Pt superlattice is shown for two different strain states of the Fe layers. The left graphs correspond to Fe with its bulk lattice spacing and the right to a strained state. Note how the envelope function merges towards a single peak. For such a superlattice structure only the mean lattice spacing, $\bar{d}$, can be extracted directly from:

$$Q_z = 2\pi \left( \frac{1}{\bar{d}} + \frac{m}{\Lambda} \right)$$

(4.9)

where $m$ is an integer describing the order of the superlattice peak relative to the main diffraction peak ($m = 0$).

The theory presented above is derived for ideal superlattices. A number of different models have been proposed to explain the lowering of satellite intensities and peak broadening effects in the diffraction pattern from real samples [33, 35–39]. Thickness variation of the layers will result in a broadening of the superlattice satellites as a function of scattering vector. Interdiffusion on the other hand will reduce the intensity of the satellites while the lineshape is unaffected. There exist numerous different models and methods to parameterize different defects of superlattice structures. One of the most simple ways is to model the integrated intensities of the superlattice lines. In doing so, effects that give broadening of the peaks are ignored, i.e. thickness variations and crystalline defects [36]. The extractable parameters are the composition profile (interface widths), the layer thicknesses and the individual lattice parameters. This route is rather simple since the integrated peak intensity can be modeled by $I(Q_z) = \langle F_{UC} \rangle \langle F_{UC} \rangle^*$ which greatly simplifies the calculation of the intensities. If the entire diffraction is to be modeled the intensity has to be calculated by $I(Q_z) = \langle FF^* \rangle$, where $F$ denotes the scattered amplitude from the entire sample [40]. Consequently, if the total intensity is to be modeled the averaging has to be made over an ensemble of superlattices with the phase included.

4.3 Reflectivity

In reflectivity the wave vector transfer is so small that length scales larger than the interatomic distances are probed. Thus, the contrast arises due to the variation in the scattering length density. This makes the method insensitive to the crystal structure. Consequently, it can be applied to any layered material from single crystalline to amorphous.

The condition for specular reflectivity is that the incident angle is the same as the exit angle. This is equivalent to that the scattering vector, $\mathbf{Q} = Q_z \hat{z}$, is perpendicular to the surface. Specular reflectivity is sensitive to the mean scattering length density profile perpendicular to the surface and can yield information about layer thicknesses, composition, density and the interface.
width. When the condition for specular reflectivity is not fulfilled there will be no specular reflected wave, instead the off-specular or diffuse reflectivity will be probed. Note that the diffusely reflected intensity also exists at the specular condition. This intensity arises solely from the roughness of the interfaces. The diffuse reflectivity contains more information about the interface quality. This can yield information about correlation lengths, jaggedness and also the separation between interdiffusion and roughness of the interfaces [41].

4.3.1 Layer Imperfection Models
All interfaces will have roughness and to some extent interdiffusion. Figure 4.3 shows schematically the difference between roughness, with a locally sharp interface, and interdiffusion, with a smooth composition variation as a function of depth. Note that the two interfaces have the same in-plane averaged composition profile, also shown in figure 4.3. In general it is difficult to achieve detailed information about the shape of the interface profile, and in most cases an error function profile is a sufficient approximation. Usually the interface width is characterized by its root mean square value, $\sigma$. For real samples there will be a contribution from both roughness, $\sigma_r$, and interdiffusion, $\sigma_i$, to the total roughness:

$$\sigma = \sqrt{\sigma_r^2 + \sigma_i^2} \quad (4.10)$$

This implies that if the total interface width can be determined, for example from x-ray reflectivity, it is necessary to determine either the width of the interdiffusion or the roughness in order to separate the two parts.
It turns out that a natural way to model interfaces is through the height-height correlation function \([42]\), defined as

\[
C(\vec{R}) = \left\langle z(\vec{r})z(\vec{r} + \vec{R}) \rightangle_{\vec{r}}
\]  

(4.11)

where \(z(\vec{r})\) is the vertical position of the interface at the in-plane position \(\vec{r}\). The brackets denote averaging over all in-plane positions. A popular choice of correlation function which has proved to capture most of the features seen in experimental data is given by \([42, 43]\)

\[
C(\vec{R}) = \sigma^2 e^{-\left(\frac{|\vec{R}|}{\xi}\right)^2 h}
\]  

(4.12)

where \(\xi\) is the in-plane correlation length of the roughness and \(h\) is the jaggedness parameter, restricted to the interval \([0, 1]\). This form of \(C(\vec{R})\) assumes an isotropic interface. \(\xi\) controls the length scale of the roughness as shown in figure 4.4. The figure shows that when \(\xi\) is lowered the length scale of the roughness is decreased. Figure 4.5 shows the effect of the jaggedness, \(h\), on the interface profile. A lower \(h\) results in a more jagged surface and a value of \(h = 1\) results in a smooth surface.

For samples with more than one interface, correlations between the different interfaces can occur. The underlying interfaces will serve as templates and some of the interface profile of the underlying layers will be replicated throughout the sample. This is described by the correlation function between interfaces \(i\) and \(j\), \(C_{i,j}(\vec{R})\). The correlation between the interfaces is usually assumed to decay exponentially with the distance between the interfaces. One possible form of the correlation function for a multilayer is \([42, 44]\)

\[
C_{i,j}(\vec{R}) = \sigma_i \sigma_j e^{-\left(|\vec{R}|/\xi\right)^2 h} e^{-|\Delta z_{i,j}|/\xi_{\perp}}
\]  

(4.13)
Figure 4.5: Example of $z(R)$ surfaces with varying jaggedness $h$ and $\xi = 300\text{Å}$.

Figure 4.6: The sample geometry assumed for Parratt’s recursive algorithm.

where $\Delta z_{i,j}$ is the distance between interface $i$ and $j$ and $\xi_\perp$ is the out-of-plane interface correlation length. This form of the correlation function assumes that all interfaces have identical $h$ and $\xi$. For a more detailed discussion about correlation functions and interfaces the reader is referred to the literature on this subject [33, 42, 43, 45–49]

4.3.2 Specular Reflectivity

Although the kinematical scattering theory as described in the previous section can be used to model the specular reflectivity it breaks down at low angles due to dynamic effects. Thus, it is necessary to include dynamical effects, i.e. refraction and multiple reflections, to correctly simulate the measured data. One way to calculate the reflectivity is by using Parratt’s recursive algorithm [33, 49, 50]. The sample is assumed to be divided into slabs on an infinite substrate as shown in figure 4.6. The wave vector transfer, $q_z$, in each layer is calculated by
\[ q_{z,j} = 2k_0 \sqrt{n_j^2 - \cos^2(\Theta)} \]  

(4.14)

where \( k_0 \) is the length of the wave vector in vacuum and \( n_j \) is the refractive index of layer \( j \). The amplitude of the reflectivity is calculated using the following recursive formula, starting with the bottom interface where the reflected amplitude is zero:

\[
R_j = \frac{R_{j+1} e^{id_j q_{z,j}} + r_{j+1,j} e^{id_{j+1} q_{z,j}}}{1 + R_{j+1} r_{j+1,j} e^{id_{j+1} q_{z,j}}} 
\]

(4.15)

\[
r_{j+1,j} = \frac{q_{z,j} - q_{z,j+1}}{q_{z,j} + q_{z,j+1}} \]

(4.16)

where \( d_j \) is the thickness of the \( j \)th slab and \( r \) is the Fresnel reflection coefficient for a single interface. The reflected intensity is obtained by \( I_R = |R|^2 I_0 \), where \( I_0 \) is the incident intensity.

To include interface imperfections, the most computationally effective way is to include a roughness factor which is multiplied with the Fresnel reflection coefficient \( r_{j,j+1} \). For an interface region with an error function profile the roughness/interdiffusion can be included by the Nevot-Croce factor \( e^{-q_{z,j}^2 \sigma_j^2/2} \) or the Debye-Waller factor \( e^{-q_{z,j}^2 \sigma_j^2/2} \). The difference between the factors is only important at small incidence angles [42, 49]. Another way to include roughness/interdiffusion is to model the imperfections by making a concentration gradient, dividing the material into thin slices with a variation in the composition across the interfaces.

### 4.3.3 Nonspecular Reflectivity

This section will present the cross-section for non-specular reflectivity calculated for multilayers in the Distorted Wave Born Approximation (DWBA) which includes dynamical effects. The kinematical treatment neglects the effects of refraction and multiple scattering. These effects are important near the critical angle of total reflection. The multiple scattering effects can also show up in the diffuse scattering for correlated interfaces of multilayers. The development of the DWBA for nonspecular reflectivity was pioneered by Shina and coworkers [43] for a single interface and later extended to multilayers by Hóly and coworkers [46, 47]. The essence of the DWBA is to use perturbation theory, where the roughness is treated as a perturbation of a perfect multilayer. The undisturbed states used in the calculations are the states corresponding to the specular reflection of the incident beam and the time inverse of the scattered beam. These states are denoted \( i \) and \( f \), respectively. The construction is shown in figure 4.7. The cross section for the diffuse scattering from a
multilayer can be written as [48, 51–53]

\[
\frac{d\sigma}{d\Omega}_{\text{diff}} = \frac{A k_0^3}{8\pi} \sum_{j=1}^{N} (n_j^2 - n_{j+1}^2)(n_k^2 - n_{k+1}^2)^* 
\times \sum_{m,n=0}^{3} \frac{e^{-\frac{1}{2}((q_{m}\sigma_j)^2 + (q_{n}\sigma_k)^2)}}{q_{m}\sigma_j(q_{n}\sigma_k)^*} G_{j}^{m} (G_{k}^{n})^* S_{j,k}^{m,n}(q_s) \tag{4.17}
\]

where the first two summations, over \( j \) and \( k \), are over all interfaces and the last two summations are over the four different scattering processes. \( A \) is the illuminated area of the sample. The factors \( G_{j}^{m} \) are calculated from the electric field amplitudes at interface \( j \) given by \( G^0 = T_T T_f \), \( G^1 = T_T R_f \), \( G^2 = R_T T_f \) and \( G^3 = R_T R_f \). The electric field amplitudes can be calculated using a recursive method similar to Parratt’s method. \( q_{m}\sigma_j \) denotes the z-component of the wave vector transfer for the scattering process \( m \) at interface \( j \). The different scattering processes are schematically shown in figure 4.8. The figure shows each scattering process as a gray ellipse, and the number used in the summation, \( m \) or \( n \), is shown above each process. It should be noted that the computation time scales with \( N^2 \) where \( N \) is the number of layers in the structure. Thus, calculations for a sample with a large number of layers are quite time consuming. \( S_{j,k}^{m,n}(q_s) \) is given by

\[
S_{j,k}^{m,n}(q_s) = \int_{-\infty}^{+\infty} \left( e^{q_{m}\sigma_j(q_{n}\sigma_k)^*} c_{j,k}(X) - 1 \right) e^{-iq_s X} dX \tag{4.18}
\]
Figure 4.9: Calculated diffuse x-ray reflectivity of a Fe/Pt superlattice with different vertical correlation lengths. The left graph is for a vertical correlation length much larger than the total thickness of the superlattice and the right corresponds to a correlation length of one third of the total thickness. The horizontal axis is the incident angle and the vertical axis the exit angle.

where \( C_{j,k}(X) \) is the height-height correlation function between interface \( j \) and \( k \). \( C_{j,k}(X) \) contains the statistical description of the interface as discussed in section 4.3.1 and an example of a possible function is equation (4.13). The Fourier transform in equation (4.18) is usually quite time consuming to calculate numerically. One approach to speed up the calculations is to Taylor expand the expression in the integral [51]. Rewriting (4.18) gives

\[
S_{m,n}^{j,k}(q_x) = \int_{-\infty}^{+\infty} \left( e^{K \exp(|X|/\xi)^{2b}} - 1 \right) e^{-iq_x X} dX
\]

(4.19)

which implies a limitation for \( C_{j,k}(X) \) to be of the form

\[
C_{j,k}(X) = Ke^{-|X|/\xi)^{2b}}
\]

(4.20)

where \( K' \) is independent of \( X \). Taylor expanding \( S_{m,n}^{j,k}(q_x) \) yields

\[
S_{m,n}^{j,k}(q_x) = \sum_{n=1}^{\infty} \frac{K^n}{n!} \frac{\xi}{n^{1/2}h} F_h \left( \frac{q_x \xi}{n^{1/2}h} \right)
\]

(4.21)

where

\[
F_h(\omega) = 2 \int_{0}^{+\infty} e^{-t^{2b}} \cos(\omega t) dt
\]

(4.22)

The function \( F_h(\omega) \) can be tabulated in advance, thus improving the calculation speed.

Figure 4.9 shows examples of calculated diffuse scattering from a Fe/Pt superlattice. The left graph shows the diffuse scattering from a completely correlated sample, whereas the right show the scattering from a sample having a
Figure 4.10: The real part, top, and imaginary part, bottom, of the scattering length of Fe at zero wave vector transfer. The unit on vertical axis corresponds to the scattering length per electron where $r_e$ is the Thomson scattering length.

correlation length of approximately one third of the total thickness. The sheets in the figure are diffuse sheets around the Bragg peaks of the multilayer. The slight bending of these sheets is due to refraction at low incident/exit angles. Also seen in the left figure are diffuse Bragg peaks at positions corresponding to the incident or exit beam satisfying the Bragg position. The effect of the vertical correlation length on the scattering pattern is seen by comparing the two graphs. The Bragg sheets become wider as the vertical correlation length is decreased. In addition, the diffuse Bragg peaks become weaker.

4.4 X-rays and Neutrons

X-rays interact with the electron cloud of the atom whereas neutrons interact with the nucleus as well as with the electrons through its spin. This difference in interaction gives different contrast in diffraction experiments. It will be explained below how this difference can be exploited to solve various questions in materials characterization. The magnetic contrast with neutrons will be discussed in section 5.3.

The scattering length for x-rays can be written as

$$f(Q,E) = f_0(Q) + f'(E) + if''(E)$$

(4.23)

Thus the total scattering length of an atom is separated into an energy independent part, $f_0(Q)$, and an energy dependent part, $f'(E) + if''(E)$. The energy dependent part is also known as dispersion corrections and arises from the fact that the electrons are bound in an atom. The total scattering length for Fe is displayed in figure 4.10. As a reference the position for CuK$_\alpha$ radiation is shown by arrows. $f_0(Q)$ depends on the scattering vector since the elec-
The electron cloud has a finite extension. In forward scattering, $Q = 0$, $f_0(0) \approx Z$ [54] where $Z$ is the number of electrons in the atom, see figure 4.11. For thermal neutrons the nuclear scattering length, $b$, is independent of the scattering vector since the extension of the nucleus is small compared to the wavelength. For neutrons it is generally not needed to take into account an energy dependent term. The scattering length of neutrons as a function of the atomic number [55] can be seen in figure 4.11. It is seen that the scattering length varies randomly with the atomic number. In the figure the positions for Fe and Co have been marked by arrows. Fe and Co being neighbors in the periodic system results in a small contrast with x-rays whereas the contrast is quite favorable with neutrons. This was exploited in paper IV to determine the composition profile of the Fe$_{82}$Ni$_{18}$/Co system. The fact that neutrons can distinguish between neighboring elements makes it a useful complement to laboratory x-ray measurements. Another advantage is that it is sensitive to light elements, such as hydrogen and oxygen, in a material containing heavy atoms.
This section will introduce the magnetic characterization techniques used in the work presented in this dissertation. The focus will be on x-ray magnetic circular dichroism (XMCD) since this is the most used method in the included papers. XMCD is measured by recording the dichroic signal with circular polarized x-rays over an absorption edge. The absorption is usually recorded by a secondary process such as electrons or fluorescent x-rays, i.e. not the change in transmitted light. For 3d metals it is most common to record the absorption with electrons since the fluorescent yield is rather low for the absorption edges of interest. The XMCD signal can be analyzed to yield the separate spin and orbital contribution for the element of interest. Thus, if the sample consists of different elements, each element's magnetic moment can be quantified. This is one of the big advantages of using XMCD. However, in order to measure XMCD a synchrotron is needed to obtain a high intensity source of polarized x-rays, which makes routine use problematic.

A technique closely related to XMCD is the magneto-optical Kerr effect (MOKE). With this technique the change of polarization and/or intensity of light reflected from the sample is recorded. The effect is particularly prominent close to absorption edges as in XMCD, see paper II. However, it is also present at optical wavelengths, making it a very useful tool for in house research. It is not possible to extract quantitative numbers of the magnetization from these measurements. Instead, relative measurements are taken, for example how the magnetization changes as a function of the applied field, i.e. hysteresis loops, or as a function of temperature.

Neutrons have a magnetic moment and thus also interact with the magnetic moment of the unpaired electrons. Using neutron reflection or diffraction gives information about the spatial distribution of the magnetic moment. This is presented in the last section.

5.1 X-ray Magnetic Circular Dichroism

X-ray magnetic circular dichroism (XMCD) was introduced in 1987, making it a relatively new technique for the characterization of magnetic materials. Although the first experiment was made at the K edge of iron [56] and produced a very small dichroic response, continued measurements at the L edges of transition metals [57] showed a huge effect, a dichroic response of about 20% of the total signal. The L edges are most preferable for studying d-band
magnetism since they involve excitations from a \( p \) core level up to the empty states of the \( d \) band. Thereby \( L \)-edge absorption probes the part of the electronic structure that is most important for magnetism in the transition metals. The \( s \) and \( p \) bands also carry a small moment although it is almost negligible compared to the high moments found in the \( d \) band.

These features together with more sophisticated analysis methods, using so-called sum rules [58, 59] (see below), laid the road to future use. With the advantages of core level x-ray absorption, its element specificity and in theory even site specificity due to the chemical shift, it has become a great tool for characterization of thin films. The sum rules also paved the way, not only for determining the orbital and spin magnetic moments of separate elements, but also for probing the anisotropic behavior of the two moments.

The fact that at the \( L_2/L_3 \) edges the deexcitation process proceeds via non-radiative processes (ejection of electrons) rather than fluorescence [54] has made XMCD very popular for surface studies, although this poses an obstacle for more bulk-like materials like superlattices. In fact, since the probing depth of electrons is rather short (on the order of 20 Å) it is an extremely surface sensitive method. Despite this disadvantage its element specificity makes it very attractive for certain problems where the magnetic moments of different elements have to be separated for the understanding of the behavior of materials.

5.1.1 The Sum Rules

A Simple Model

Circular dichroism is a phenomenon arising from the fact that a photon transfers its angular momentum (\( \pm 1 \)) to an absorber which is sensitive to the change in angular momentum (change in polarization). An angular momentum of \( \pm 1 \) corresponds to left/right handed circular light. So, for example, if only electronic transitions with \( \Delta m = \pm 1 \) are to be probed the incident light has to be left/right handed circular. This is the reason why circular polarization is used when probing the magnetic moment with XMCD. If, on the other hand, linearly polarized light is used, the photon will carry an average angular momentum of zero since linearly polarized light is a superposition of right and left circular light with equal weights.

In this section a simple model that explains the basic mechanism behind the XMCD effect at the \( L_2 \) and \( L_3 \) edges will be shown. Examples of iron spectra are shown in figure 5.1. The following explanation of magnetic dichroism mainly follows the two-step model from Kapusta and coworkers [60] and is explained in more detail by Lovesey [61].

The two-step model separates the excitation process in two steps, see figure 5.2. In the first step the electrons are excited from the ground state to an unoccupied band (in this case a \( d \) band). Next, the final state works as a filter for the excited electrons. This implies that if the current experiences a spin and/or
orbital polarization it will be sensitive to the corresponding polarization of the final state.

As stated above it is quite intuitive that the XMCD effect is orbital sensitive, since upon absorption the orbital quantum number \((m_l)\) for an electron changes by \(\pm 1\). The ability to also probe the number of unoccupied spin states stems from the fact that the 2p core level experiences spin-orbit splitting. This effect comes from the coupling between the spin and the angular momentum. The consequences are that the 2p level splits into a 2p\(_{1/2}\) and a 2p\(_{3/2}\) state, and the spin and angular momenta of the electrons will be coupled. For the 2p\(_{1/2}\) and 2p\(_{3/2}\) levels they will be coupled parallel and antiparallel, respectively. This is the basis of the possibility of obtaining information about the spin magnetic moment.

To understand how it is possible to separate the spin and orbital moments a more detailed picture than the qualitative view given above is needed. In order to do this the expectation values of the spin, \(\langle s \rangle\), and orbital momentum, \(\langle l \rangle\), of an electron excited to an empty d band are needed. The expectation value multiplied by the density of empty states, \(\rho\), is proportional to the absorption coefficient. The connection between absorption coefficient, \(\mu^\pm\), and the above parameters can be written as [61]

\[
\mu^\pm(E) = \mu_0(E) \pm \mu_m(E) \propto \rho \pm A\langle s \rangle \Delta \rho_s(E) \pm B\langle l \rangle \Delta \rho_l(E)
\]  

(5.1)

where \(\pm\) refers to the photon angular momentum, \(\mu_0(E)\) is the non-dichroic part of \(\mu^\pm\) and \(\mu_m\) is the dichroic part of the absorption coefficient. All that
Figure 5.2: The two-step model of spin dependent absorption. A photon excites an 
electron from the 2p core level. If these photons exhibit spin polarization it is possible 
to probe the difference in spin up and spin down holes.

<table>
<thead>
<tr>
<th>Edge</th>
<th>⟨s⟩</th>
<th>⟨l⟩</th>
<th>N</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_3$ 2$p_{3/2}$</td>
<td>$1/8$</td>
<td>$+3/2$</td>
<td>$4$</td>
</tr>
<tr>
<td>$L_2$ 2$p_{1/2}$</td>
<td>$-1/4$</td>
<td>$+3/2$</td>
<td>$2$</td>
</tr>
</tbody>
</table>

Table 5.1: Expectation values for the spin, ⟨s⟩, and orbital, ⟨l⟩, momentum of the elec-
tron when excited to an empty d-band. N is the number of electrons in the respective 
core-level. The values refer to a photon angular momentum of +1.

is needed now is the expectation values of the excited electrons. This can 
be calculated from the transition probabilities of each excitation. In table 5.1 
the values are reproduced from [60, 61]. From this table we can see that 
the expectation value for ⟨l⟩ is constant for the $L_2$ and $L_3$ edge and that ⟨s⟩ 
changes sign when going from the $L_2$ to the $L_3$ edges. One interesting exercise 
is to calculate the expectation value of the spin for both edges. The total value 
will be

$$\langle s \rangle(p_{1/2}, p_{3/2}) = \frac{2 \times \frac{1}{4} + 4 \times \frac{1}{8}}{2 + 4} = 0$$

(5.2)

This means that in the absence of spin-orbit coupling there will be no spin 
polarization, which also applies to the integral over the $L_2$ and $L_3$ edges of 
the difference in absorption between left and right circularly polarized light. 
At the same time, if the area of the $L_2$ difference is subtracted from the area 
of the $L_3$ with correct weighting, it will be proportional to the spin moment. 
These rather simple arguments can be followed and sum rules for the two-
step model can be extracted. However, these sum rules will differ from more 
realistic atomic calculations [58, 59] that will be reviewed in the next section.
The Sum Rules

The sum rules as derived by Thole and Carra [58, 59] relate the integrated difference in absorption between left and right handed circularly polarized light to the orbital and spin magnetic moment. The absorption coefficient can be written as

$$\mu^\pm(E) = \mu_0(E) \pm \mu_m(E)$$  \hspace{1cm} (5.3)

The ± refers to right and left handed circularly polarized light, respectively. The XMCD integrals over the \(L_2\) and \(L_3\) peaks are defined as

$$\Delta L_3 = \int_{L_3} (\mu^+(E) - \mu^-(E)) dE$$  \hspace{1cm} (5.4)

$$\Delta L_2 = \int_{L_2} (\mu^+(E) - \mu^-(E)) dE$$  \hspace{1cm} (5.5)

where \(E\) is the energy of the incoming photon. Using these definitions the orbital, \(m_l\), and spin, \(m_s\), magnetic moments of the probed atom can be analyzed by [58, 59]

$$\Delta L_3 + \Delta L_2 = -\frac{C}{2\mu_B} m_l$$  \hspace{1cm} (5.6)

$$\Delta L_3 - 2\Delta L_2 = -\frac{C}{3\mu_B} (m_s - m_D)$$  \hspace{1cm} (5.7)

The constant \(C\) is usually taken as an element specific constant [62]. In the strict sense it contains the polarization of the photons, and the number of holes per unit area. \(m_D\) is the anisotropic part of the spin moment, usually called the dipole moment.

Although the sum rules at a glance seem to be able to give the spin and orbital moments directly it is generally agreed [62–64] that the sum rules should be used for relative measurements. This will be discussed further in the next section.

Saturation Effects

Saturation effects are usually discussed in the conjunction of x-ray absorption spectroscopy when the absorption is detected by secondary processes, such as fluorescence or electron yield. The term refers to that the signal detected is not proportional to the absorption coefficient in the sample studied. This can affect the determination of integrals which is crucial to the sum rule analysis. For XMCD measurements this subject has been treated by a number of authors [63–65].

First of all the electron yield created by a photon is directly proportional to the absorption [65]. The saturation effect originates from that as the photon beam travels into the sample it will be absorbed and thereby the intensity at a certain depth will vary as a function of energy. This, combined with the limited mean free path of the electrons, can saturate the spectrum under certain
Figure 5.3: A picture of the length scales involved in saturating the electron yield.

circumstances that will be dwelled upon in the following discussion. A picture of the process can be seen in figure 5.3, which also defines the different variables. The intensity at a depth \( z \) can be written as

\[
I(E, z) = I_0 e^{-\frac{\mu z}{\cos \theta}}
\]

(5.8)

where \( I_0 \) is the incident intensity and \( \mu \) is the absorption coefficient of the photons. Before the \( L_3 \) edge the photon will have a mean free path, \( \lambda_x = 1/\mu \), of about 6000 Å, which is to be reduced to approximately 200 Å at the \( L_3 \) edge. The electron yield created at a certain depth \( z \), \( dY_{e,0}(z) \), can then be calculated:

\[
dY_{e,0}(z) = I(E, z) \frac{\mu}{\cos \theta} \, dz = I_0 e^{-\frac{\mu z}{\cos \theta}} \frac{\mu}{\cos \theta} \, dz
\]

(5.9)

The electrons must travel a distance \( z \) to be detected and during their travel they will be absorbed. Taking this into account the yield at the surface from a layer at depth \( z \) will be

\[
dY_e(z) = dY_{e,0}(z) e^{-z/\lambda_e} = I_0 e^{-z(\frac{\mu}{\cos \theta} + \frac{1}{\lambda_e})} \, dz
\]

(5.10)

where \( \lambda_e \) is the mean free path of the electron, on the order of 20 Å. The total electron yield from a sample of thickness \( t \) can be calculated by integrating the above equation from 0 to \( t \).

\[
Y_e(t) = C \frac{\lambda_e}{\cos \theta} \frac{1}{1 + \frac{\lambda_e \mu}{\cos \theta}} \left\{ 1 - e^{-t(\mu/\cos \theta + 1/\lambda_e)} \right\} \mu
\]

(5.11)

This function is a nonlinear function of \( \mu \) and can therefore not be solved analytically, but it can be solved numerically. An example of the saturation in a rather extreme case and a correction of the calculated spectrum can be seen in figure 5.4. It should be noted that the most crucial thing is that the \( L_2 \) and \( L_3 \) peaks have changed areas with respect to each other. This will influence the determination of the orbital and spin moments.
Figure 5.4: The effect of electron yield saturation for an extreme case, incidence angle $\theta = 80^\circ$ and thickness $t = 40$ Å, for a Fe film (circles). Note that the $L_2$ and $L_3$ peaks have different degrees of saturation and that the correction (squares) can fully recover the true spectrum (full line).
Equation (5.11) can also be extended to multilayers. The expression below holds for a multilayer consisting of two layers, denoted as $A$ and $B$, with $N$ repetitions, but can easily be extended to any number of repeating layers:

$$Y_{e,SL} = \frac{e^{\Lambda g} - e^{-\Lambda g N}}{e^{\Lambda g} - 1} \times \left(Y_{e,A} + Y_{e,B}e^{-\mu_{A}/\cos \theta} e^{-t_A/\lambda} \right)$$

(5.12)

where $\Lambda = t_A + t_B$ is the total thickness of the repeating bilayer. $Y_{e,X}$ is given by equation (5.11) with the constants for the respective materials inserted as $X$. The factor $g$ is given by

$$g = \frac{t_A}{\Lambda} \left( \frac{1}{\lambda_{e,A}} + \frac{\mu_A}{\cos \theta} \right) + \frac{t_B}{\Lambda} \left( \frac{1}{\lambda_{e,B}} + \frac{\mu_B}{\cos \theta} \right)$$

(5.13)

These equations have been used to test the validity of the analysis in paper I and it was found that by normalizing all values to the spin and orbital values separately to a bulk reference gave the same result as using the above corrections to within $0.1 \mu_B$. Although this section has dealt with the correction of spectra as an artifact of the measurements, they may be viewed as an opportunity instead of a limitation. Actually, Amemiya and coworkers [66, 67] have exploited this effect to obtain magnetic moment depth profiles of Cu at various interfaces by detecting the electron yield at different angles.

### 5.2 MOKE

The magneto-optical Kerr effect (MOKE) has the same microscopic origin as XMCD. The angular moment of the light interacts with the orbital moment of the electrons which is coupled to the spin through the spin-orbit interaction. However, since most MOKE experiments are conducted with visible light with a rather low energy compared to soft x-rays, the excitations originate in the high-lying conduction bands. Therefore, there exist no sum rules for quantification of the measurements. Instead MOKE is usually used to record hysteresis loops of magnetic films. It has also other uses, for example recording the change in magnetization versus temperature. Since MOKE is an optical technique it has a finite probing depth. For a good conductor, like metals, it is in the order of $100 \, \text{Å}$ [68]. Thus, it is not as surface sensitive as XMCD measured in electron yield.

Three different geometries are usually discussed for the Kerr effect depending on the relative orientation between the incident light and the magnetization. The geometries are shown in figure 5.5. The longitudinal effect and the polar effect will rotate the plane of polarization and induce an ellipticity of the reflected light. Usually, the polar effect is larger than the longitudinal effect [69]. The transverse effect will only change the intensity of the reflected light. These effects also depend on the angle of incidence. For the polar effect the response is largest at normal incidence. At the same time, for normally
incident light, there is no MOKE response for the longitudinal and transverse effects.

To calculate the magneto-optical response of a multilayer structure Zak and coworkers [70–73] developed a macroscopic formalism based on medium boundary and propagation matrices. Given the optical constants, both isotropic and magneto-optical, and the orientation of the magnetic moments it is possible to calculate the reflection coefficients. This formalism can also be applied to x-ray resonant magnetic reflectivity [74]. It should be noted that Zak’s formalism yields the same results as the theory presented in paper II.

For detailed discussions about MOKE the reader is referred to the reviews found in [69, 75, 76]. Also, a description about the various experimental configurations can be found in [77].

5.3 Neutron Scattering

Since the neutron has a magnetic moment it will interact with the electronic magnetic moment distribution. Thus, diffraction of neutrons from a magnetic crystal allows determination of the distribution and directions of the magnetic moments. The refinement of the magnetic structure using neutron diffraction is today a well established technique. In the same manner the magnetic distribution and directions in thin films can be probed with neutron reflectometry [78–80]. Since this thesis involves a rather limited amount of work with neutron diffraction only a brief introduction to the subject will be given as a background for paper IV. The presentation given in this section is based on textbooks on neutron scattering [81, 82], where more information can be found.

The structure factor including both nuclear and magnetic scattering can be written as [82]

\[ F^2 = F_N^2 + 2F_N F_M \vec{q} \cdot \vec{P} + q^2 F_M^2 \]  \hspace{1cm} (5.14)

where \( F_N \) is the nuclear structure factor and \( F_M \) is the magnetic structure factor. These structure factors are calculated according to equation 4.3 with the coherent nuclear scattering length, \( b \), inserted for \( F_N \) and the magnetic scat-
The nuclear scattering length, \( p \), for \( F_M \). As discussed in section 4.4 the nuclear scattering length is independent of the scattering vector due to the small size of the nucleus compared to the wavelength of the neutron. For magnetic scattering the neutron scatters off the electronic magnetic moment distribution which has an extension of the order of the atomic size. Thus, the magnetic scattering length will depend on the scattering vector, similar to x-rays. \( \vec{P} \) is a unit vector in the direction of the neutron polarization and \( \vec{q} \) is the magnetic interaction vector defined as

\[
\vec{q} = \vec{\kappa} (\vec{\kappa} \cdot \vec{\eta}) - \vec{\eta}
\]

(5.15)

where \( \vec{\kappa} \) is a unit vector parallel to the scattering vector and \( \vec{\eta} \) is a unit vector in the direction of the magnetization. The different vectors are also shown in figure 5.6. For an unpolarized neutron beam \( F^2 \) will become

\[
F^2 = F_N^2 + q^2 F_M^2
\]

(5.16)

Thus, the cross term between the magnetic and nuclear scattering disappears. The prefactor \( q^2 \) in front of the magnetic structure factor is

\[
q^2 = 1 - (\vec{\kappa} \cdot \vec{\eta})^2 = \sin^2 \alpha
\]

(5.17)

where \( \alpha \) is the angle between the scattering vector and the magnetization vector. If the magnetization of the sample is parallel to the scattering vector, \( q^2 = 0 \), there will be no magnetic scattering.
6. Summary of Results

This chapter reviews the results and conclusions from the papers presented in this dissertation. The backgrounds to the methods used have been reviewed in the previous chapters and the detailed experimental procedures are described in the articles. The chapter starts by discussing the influence on the magnetic moment of the interface structure. It will then shift focus to the influence of strain on the magnetocrystalline anisotropy. Lastly, some conclusions from the work presented here are given.

6.1 Magnetic Moments and Interfaces

The change of the spin magnetic moment in superlattices with respect to the bulk is largely determined by the interfaces. Also, as has been shown by Holmström and coworkers [25] the degree of interdiffusion is the main controlling parameter for the spin magnetic moment in Fe/V superlattices. Since superlattices consist of at least two elements it is not always sufficient to conduct measurements of the mean magnetic moment. In order to reveal the more detailed behavior of the magnetic moments the measurements have to be conducted with element specificity, i.e. XMCD, and/or with a depth resolved probe, e.g. neutron reflectivity and x-ray resonant magnetic reflectivity (XRMR).

For both the Fe/Co [17] and the Fe_{0.82}Ni_{0.18}/Co [1, 83] systems the magnetic moment dependence on the individual thicknesses showed a rather unexpected behavior in previous studies. For the Fe/Co system the conclusion from a combined neutron reflectivity and SQUID study indicated that the Co moment was enhanced to \(2.1 \mu_B/\text{atom}\) in the two layers closest to the interface, while the Fe had an enhanced region of 4ML (monolayers) with a maximum moment of \(3.0 \mu_B/\text{atom}\), which corresponds to an enhancement of \(0.8 \mu_B/\text{atom}\) relative the bulk moment. For the Fe_{0.82}Ni_{0.18}/Co system previous SQUID measurements showed a region of enhancement of 3.5ML at the interfaces with an enhancement of about \(0.3 \mu_B/\text{atom}\).

The bcc Fe/Co (001) superlattices were studied with XMCD in paper I and with XRMR in paper II. The XMCD results showed that the Co moment remained at its bulk value of \(1.6 \mu_B/\text{atom}\) and that the Fe moment showed a large region of enhancement with a magnetic moment of \(3.0 \mu_B/\text{atom}\) in the atomic layer closest to the interface. In addition, the Fe moment also showed some dependence on the Co thickness. For small Co thicknesses the Fe moment was found to decrease relative to samples with thicker Co layers. The explanation
Put forward for the dependence on the Co thickness was that, for a critical thickness of the Co layer, the Fe atoms start to be affected by the preceding Fe layer instead of the Co layer. XRMR measurements on a sample with 6 ML Fe and 6 ML Co showed that even the interior region of the Fe layer has an enhanced moment. More recent theoretical calculations by Bergman and coworkers [84] reproduce the trend as well as the magnitude of the Co moment. However, the magnitude and the region of enhancement of the Fe moment are not reproduced by the calculation. The discrepancy between theory and experiments could be explained by a large amount of interdiffusion. There are strong indications that a significant amount of interdiffusion exists in these types of structures [85]. Motivated by these measurements Wieldraaijer and coworkers [86] measured $^{59}$Co nuclear magnetic resonance on a 6 ML Fe/6 ML Co superlattice and found that about 25% of the Co was surrounded by Co only. Thus, interdiffusion and island growth [5] of the bcc Co is a highly probable cause for the observed trend in the previous studies.

For the bcc Fe$_{0.82}$Ni$_{0.18}$/Co (001) superlattices special attention was paid to the interface region in order to resolve the detailed magnetic moment profile in this system, see paper III. As mentioned above, the region of enhancement of the magnetic moment had previously been determined to be 3.5 ML. Thus, a series of sample was grown to study the influence of the FeNi layer thickness (2-6 ML) as well as the Co layer thickness (2-6 ML) while keeping the other element constant at 6 ML. The element specific magnetic moments were studied with XMCD. The behavior of the Co moment was, as expected, constant as a function of thickness and close to its bulk value. However, even the Fe moment was found to be constant at about 2.8 $\mu_B$/atom for the entire thickness range studied. These findings were compared to ab initio calculations which pointed out that the entire layers had to be interdiffused in order to reproduce the size of the moment for the series studied here. In doing the calculations it was assumed that the interdiffused layers formed an ordered B2-type alloy [87] (CsCl structure [88]).

To resolve whether or not any appreciable B2 ordering existed, neutron diffraction measurements of two samples, Fe$_{0.82}$Ni$_{0.18}$3 ML/Co3 ML and Fe$_{0.82}$Ni$_{0.18}$12 ML/Co12 ML, were conducted. The Fe$_{0.82}$Ni$_{0.18}$3 ML/Co3 ML sample was used to resolve any B2 ordering since it should consist entirely of interfaces, and the Fe$_{0.82}$Ni$_{0.18}$12 ML/Co12 ML was used to determine the composition profile. As described in section 4.4, the contrast between Fe and Co is low for x-rays but excellent with neutrons. From the neutron measurements it was seen that no appreciable long range B2 ordering was present. However, from the co-refinements of x-ray and neutron data on the Fe$_{0.82}$Ni$_{0.18}$12 ML/Co12 ML sample it was possible to extract the interface widths. This showed two very different interfaces, see figure 6.1. One interface has a total interface width of 10 ML and the other interface is close to perfect with a maximum total width of 1 ML. Comparing this with the discussion on the Fe/Co system the
FeNi-on-Co interface should be interdiffused and thus give the large region of magnetic moment enhancement.

6.2 Magnetism and Strain

The spin part of the magnetic moment is usually quite insensitive to moderate strains. However, the orbital moment is usually said to be highly sensitive to strain especially in 3$d$ metals where the orbital moment is quenched. Also, the magnetocrystalline anisotropy shows a significant dependence on the strain: the magnetoelastic effect.

In connection to the dependence of magnetocrystalline anisotropy on strain, Burkert and coworkers [7] made a theoretical study of the dependence of the uniaxial magnetocrystalline anisotropy in FeCo alloys on the composition and strain, as characterized by the $c/a$ ratio. It was found that FeCo alloys have a maximum in the uniaxial anisotropy, $K_u \approx 700 \mu$eV/atom, for a $c/a$ ratio of 1.20–1.25 and a composition of about 60 at. % Co. This high value of the magnetocrystalline anisotropy can be found in other materials as well such as the ordered FePt alloys [7], but the predicted high magnetic moment of these alloys, $2.1 \mu_B$/atom, makes it a technologically interesting material for magnetic recording applications. This motivated the study presented in papers V–VIII. In order to induce the high strains necessary to reach the desired $c/a$ ratio, Pt was chosen as a spacer layer between the FeCo alloy layers. The Co concentration of the FeCo layers was chosen to be as close as possible to the theoretical optimum 60 at. %.

In paper V the initial results of the structural and magnetic characterization are presented together with a comparison to theoretical results. These results showed that the samples as produced by sputtering have the right $c/a$ ratio, determined by x-ray diffraction, and the right stoichiometry ($64 \pm 5$ atomic %), as determined by x-ray photoelectron spectroscopy and Rutherford backscat-
Figure 6.2: The mean in-plane lattice parameter for some of the studied samples. The dashed lines are bulk lattice parameters for the indicated materials. The full line represents an fcc Fe$_x$Pt$_{1-x}$ alloy.

tering. However, the uniaxial magnetocrystalline anisotropy was about one fourth of the theoretical expected maximum. The detailed characterization of the magnetocrystalline anisotropy can be found in paper VII where the strain and interface contribution to $K_u$ was studied. The interface contribution in this paper was modeled with equation (3.14) and the strain contribution was modeled to be quadratic in $c/a$ to give a zero contribution for the $c/a$ ratios corresponding to the bcc and fcc structures. It was found that the strain gives a sizeable contribution to the magnetocrystalline anisotropy.

The detailed structural characterization of these samples is presented in paper VI. The emphasis is on the determination of the $c/a$ ratio from the x-ray diffraction patterns. A simple model for directly calculating the individual lattice parameters for the FeCo alloy from the mean lattice parameters is presented by assuming a volume preserving response and no relaxation of the lattice parameters within each layer. This is compared with simulations of the x-ray diffraction pattern around the (002) reflection. Also, the experimentally derived $c/a$ ratios are compared to density functional calculations. Both the x-ray simulations and the calculations are in good agreement with the presented model. One puzzling piece of information from these measurements is that the mean in-plane lattice parameter, see figure 6.2, is smaller than both the bulk bcc FeCo alloy and bulk Pt. As can be seen from the figure, there are two possible causes: the stabilization of an fcc FeCo alloy at the interfaces or the presence of some interdiffusion at the interfaces, with formation of an FeCoPt alloy. Both of these scenarios would yield a lower in-plane lattice parameter than that expected from the constituents alone. Studying the surface segregation energies reveal that both Fe and Co show a tendency to form surface alloys on Pt, which is an indication that the second alternative could be probable. However, the degree of interdiffusion should not be too extensive since x-ray reflectivity simulations show rather well defined interfaces with an in-
terface width of 2.6 and 1.3 Å, rms values, as shown in figure 6.3. Thus, this brings back the questions raised for the Fe/Co and Fe$_{0.82}$Ni$_{0.18}$/Co systems: are the interfaces interdiffused or not?

Returning to the title of this section — magnetism and structure — leads to the results presented in paper IX, which is a study of the orbital moment’s dependence on interfaces and strain. The motivation for this project was twofold: earlier studies by Scherz and coworkers on Fe/V superlattices [20] found a constant Fe orbital moment for a series of samples. This was attributed to a competition between a strain contribution and an interface contribution. Also, there are very few experimental studies on the influence of strain on the orbital moment. Superlattice structures offer a convenient way to vary the strain while keeping the interface contribution constant for one element. This can be accomplished by simply varying the thickness of the other constituent. The results presented in paper IX, and reproduced in figure 6.4, show that there is indeed a negative contribution to the orbital moment of Fe from the interfaces, and a positive contribution from the lowering of the symmetry, i.e. increasing strain in the layer.

The FeCo/Pt system also shows interesting behavior of the orbital moment as presented in paper VIII. In these XMCD studies it is seen that the spin part of the magnetic shows the same relative decrease at the interfaces for both Fe and Co, in the studied thickness range of 4 – 10ML. The in-plane orbital moment for Co does not show a significant change at the interface whereas the Fe orbital moment shows a strong decrease. A similar trend for the Co orbital moment has been seen Au/Co/Au trilayers [89]. In that system the out-of-plane orbital moment becomes enhanced at the interfaces whereas the in-plane orbital is constant. The Au/Co/Au system also shows a spin reorientation for low Co thicknesses as the FeCo/Pt system. In addition the induced Pt magnetic moment was quantified with complementary measurements of the
Figure 6.4: The orbital moment of the studied Fe/V samples. The graph shows the dependence of the orbital moment on the thickness of the Fe layer. The inset shows the orbital moment of Fe for varying strain.

6.3 Conclusions and Outlook

The major conclusion from the work presented in this dissertation is the importance of a rigorous structural characterization of the samples in connection to the study of physical properties of interest. Perhaps one of the most demanding tasks in obtaining the structural information from scattering methods such as reflectivity and diffraction is the refinement of the assumed model to the measured data. Most ordinary fitting routines, such as Levenberg-Marquardt and the Simplex method, are local methods. This means that the physicist has to manually refine the parameters until a good fit is achieved before using the fitting routines. However, during the last decade a new, very promising, method has been developed, namely the differential evolution algorithm [90]. The main advantage with this routine is that it avoids local minima effectively and has high success rate in finding the global minimum for a wide range of problems [31, 32, 90]. This was used in paper VI to refine both the x-ray diffraction as well as the x-ray reflectivity data. In view of its usefulness a complete computer program for refining x-ray reflectivity has been developed and is presented in the appendix and paper X.

One special point is the characterization of interdiffusion which has been an issue in almost all the work presented here. Off-specular reflectivity, as
discussed in chapter 4, seems at first glance to provide an opportunity to resolve this since the signal originates only from the roughness. However, since the two contributions are added in square, see eq. 4.10, it is rather difficult to achieve a good estimation from this type of measurements. In addition, there is a high degree of correlation between the different parameters and it is difficult to achieve quantitative numbers. In this context the local probes should be mentioned, such as NMR [91], Mössbauer spectroscopy [92] and extended absorption fine structure (EXAFS) [93]. Using these techniques it is possible to extract the coordination number, under certain conditions, for different elements.

To improve the characterization of the atomic structure of the superlattice a natural extension would be to measure and refine not only the specular signal but a complete reciprocal space map. This should yield a much better understanding of the internal structure such as relaxations in the layers.

In summary, this dissertation has highlighted the need of conducting detailed structural characterization in parallel to magnetic studies on superlattice systems. This approach, naturally, yields a deeper understanding of the phenomena originating in the materials. Also, the use of the right probe has been shown, as in paper IV, to be very important in order to draw significant conclusions from the data. An active search for new and improved methods to study these types of nanoscale materials structurally will lead to a more fundamental understanding of their properties.
7. Acknowledgments

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Manual for GenX

Introduction

This manual is intended as an introduction to the GenX program. The program is an implementation of the Differential Evolution algorithm for constrained fitting of a general function to data. The Differential Evolution algorithm [31, 90] has proven to be a robust method for multidimensional optimization of non-linear functions.

Separating the function to be fitted and the model makes it readily extensible to many problems. At present it has been used to fit x-ray reflectivity and diffraction data. The models are written in the script language Python together with the SciPy package. Using an interpreting language makes the program a bit slower than a compilable programming language such as C, but instead it permits a fast implementation of new ideas. The main idea of the program is to provide a flexible and extensible environment for fitting a model to data.

The manual starts with an explanation of the user interface. It continues by explaining how to write models. Finally it briefly explains how to use the existing package for simulating x-ray reflectivity.

Installation

The program will run on all operating systems on which Python and wxPython is implemented. These are at present, according to wxPython homepage: 32-bit Microsoft Windows, most Unix or Unix-like systems, and Macintosh OS X. Currently GenX has been tested on Windows XP, Mac OS X and Linux. To install the program the following Python components need to be installed:

- Python 2.3.5, www.python.org
- SciPy 0.3.2, www.scipy.org
- Numeric 23.5, numpy.scipy.org
- wxPython 2.6, www.wxpython.org

The versions in this list are the most up-to-date versions the program has been tested with. For Windows user there exists a package called Python Enthought Edition, code.enthought.com, which contains all the packages mentioned in the list above and even some more. It should be said that SciPy might need to be reinstalled on top of that installation to get it working properly.
When all the packages are installed. Unzip the program and run the file `GenX.py` with the Python interpreter. For Windows users it should be enough to double click on the file.

The User Interface
This section will briefly explain what the different menus and buttons in the user interface do.

Main window
The main window, figure 1, is controlled by menus at the top of the window or using the buttons on the toolbar. There are also different plot folders which are chosen by clicking on the respective folder at the bottom of the window.

File menu
Open Session This opens a previously saved session. The user is asked to give a file with the extension *.dbm and the session file contains the values in the Parameters window, the data and a path to the Python file containing the model. The command also loads the model file. The path
in the session file is relative to the session file, i.e. moving the model file relative to the session file will make it unloadable\(^1\).

**Save Session**  This saves the current session, see Open session.

**Load Data**  Opens a window for importing and processing data. See section Data window.

**Load Model**  This loads a Python file that should contain the model. The Python file will be executed in the global namespace. Any errors during the execution will be reported. In addition the file must contain a function called `Sim` which takes a data structure as argument and returns a list of calculated values. See section Making a Model for more details.

**Export Data**  This exports the data to a three-column format. The first column is the x-data and the two remaining columns is the loaded data and the simulation, respectively.

**Page Setup**  Opens a dialog box for setting up the printing. These changes only apply to the printing of the different plots.

**Print Preview**  Print a preview of the graph in the active tab.

**Print**  Prints the active graph in the notebook. Uses the settings defined in Page Setup.

**Print Parameters**  Prints the parameters from the Parameters window as a spreadsheet. This does not use the settings in Page Setup.

**Exit**  Exits the program.

**Windows Menu**
This menu controls the auxiliary windows used for creating the model, loading the data and defining the parameters.

**Edit**  Opens an editor. Its main use is to edit the model file. It should be noted that saving the file only saves the file and does not load the model into the program. This has to be done using Load Model in the file menu or the button on the toolbar.

**Parameters**  Opens the Parameter window. This window defines which parameters should be fitted and their minimum values, maximum values and the start/refined value. See section Parameter window.

**Data**  Opens a window for importing and processing data. See section Data window.

---

\(^1\)Note that it is possible to load a broken file by first loading the model file, then opening the session and after that loading the model again. This makes it possible to load moved sessions and relink the model file.
Fit Menu
This menu controls the fitting process.

Start  Starts and initializes the fitting. Initialization means that any changes made in the Parameter window are transferred to the fitting algorithm. It will also create a new (random) population of parameter vectors.

Stop   Stops the fitting.

Resume Resumes the fit without the initialization. The fitting will proceed with the same population. Note that if the minimum and maximum values in the spreadsheet has changed it will not be loaded into the fitting routine.

Misc Menu
Nice Graph  This is intended for producing publication quality plots. Using this requires the package matplotlib, matplotlib.sourceforge.net.

Enable Zoom  Turns the zoom on and off in the active plot in the notebook.

About..  Shows some information about the program.

The Toolbar
The toolbar allows fast access to the functions most used. The description that follows lists the different buttons starting from the left.

Open Session  Opens a Session. See description in the File menu.

Save Session  Saves a Session. See description in the File menu.

Data  Opens the Data window.

Load Model  Loads a model. See description in the File menu.

Edit  Opens the editor. See description in the File menu.

Reload Model  Reloads the model file.

Parameters  Shows the parameter window.

Start  Starts the fitting. See description in the Fit menu.

Stop  Stops the fitting. See description in the Fit menu.

Resume  Resumes the fitting. See description in the Fit menu.

Choice list  Changes the y-axis scale. The different scaling functions are defined in the file Settings.py

Line/Points  Changes between lines and points for plotting the data.

Enable Zoom  Enables the zoom. See description in the Misc menu.
The Plots
In the bottom of the window there are several different tabs, see figure 1, that are used to display the data produced by the fitting routine. They are chosen by clicking on the respective tab.

Data Plot to show the data and the simulation. The scale of the y-axis is changed by the choice list in the toolbar. The red line corresponds to the data and the blue is the simulation. This plot is updated after every iteration/generation.

Error The plot, see figure 2, shows the evolution of the Figure of Merit (FOM) as a function of the iteration/generation.

Parameters The y-axis corresponds to the normalized parameter space. The plot, see figure 3, shows the best value of each parameter, red dot, and the maximum and minimum of the parameter in the population, blue bar. Each parameter has its own red dot and blue bar, and the x-axis correspond to the row number in the spreadsheet. A normalized parameter space means that the plot is normalized between 0 and 1 where 0 is the minimum allowed value for the parameter and 1 is the maximum allowed value. This is quite useful during fitting since it allows the user to check that the minimum and maximum values do not limit the fitting routine. It can also be used for seeing how fast certain parameters converge. In addition, it can be used to determine that all the parameters
Figure 3: A picture of the Parameters plot. Red dots represent the best value so far and blue bars represent the population spread. See text for details.

have converged, i.e. when the blue bars have vanished or are small. In that case more generations/iterations will not improve the fit.

**Escan** This plot is used by the Escan button in the parameter window. It is used to display the dependence of the error function on one parameter. The y-axis corresponds to the error function and the x-axis to the parameter value which is represented by a blue line. The point that corresponds to the value in the grid is represented by a red dot and a red line is also included to indicate a 5% increase in the errorfunction. See the section for the parameter window for more details and figure 5.

**Parameter Window**

The parameter window, figure 4, is used for defining which parameters are to be fitted and for setting the allowed minimum values, maximum values and the best guess values. It also contains some additional functions such as simulation of the values and scanning of a parameter.

**The Spreadsheet**

The spreadsheet consists of 5 columns and an arbitrary number of rows. Each row represents one parameter and the values associated with it. The first row defines the parameter by a function that sets the parameter. This function has to take a single float number as input. The use of a function instead of supplying a parameter may seem a bit tedious, but it improves the flexibility and makes
Figure 4: The parameter window with the spreadsheet and the buttons at the bottom.

less room for hard to find reference errors in the programming. Also, if the right mouse button is clicked on a cell in the first column a pop-up menu will appear allowing the user to choose from member functions in the Layer, Stack, Sample and Instrument objects defined in the model file\(^2\). The second column, Value, represents the first guess value as well as the best fit value supplied by the fitting algorithm. The third column, Fit, is a tick box. If this is ticked the parameter will be fitted. The fourth and fifth columns contain the allowed minimum and maximum values the parameter is allowed to take. The rows in the spreadsheet grows automatically as soon as the last row has a value.

If the first column is left blank the program will ignore the line. But if there is something written, and it is not a python object the program will give an error message in the form of a dialog box. Also when starting the fit all the variables (functions) in the spreadsheet are set to the corresponding value in the Value column whether or not the tick box in the Fit column is ticked.

**Buttons**

At present there are three buttons at the bottom of the window for extra functions, see figure 4. The first from the left is Simulate. This executes a simulation by first setting all the parameters defined to the value in the value column. Then it calls the Sim function and plots the simulation together with the data.

The second button is the Escan button. This will scan a selected parameter and plot the FOM versus the parameter value. The limits of the scan are determined by the minimum and maximum values. Before the FOM function is

\(^2\)Note that user defined functions have to be entered manually
scanned all the defined parameters will be set to the values in Value column. The output is plotted in the Escan folder of the notebook. Before clicking on the Escan button a row has to be selected by clicking on the row numbering to the right of the spreadsheet, see figure 4. This function can be used to estimate the uncertainty of the fit by using the above mentioned 5% level. However, this needs a word of caution: it is not the uncertainty in the parameter that is measured, since it is only a one-dimensional scan through the parameter space! If a correlation between the parameters exists, and it most probably does, this method will give a wrong number for the uncertainty.

The third button, Eproject, works similar to the Escan button. It will plot all evaluated FOM values from the fitting algorithm as a function of the selected parameter. It can be used to view the projected FOM as a function of one parameter.

Data Window
The data window represents a collection of routines for loading and processing of the data. The data that can be loaded is column based ASCII data. The program also supports the loading of multiple data sets. This can be used to fit multiple data sets or to cut out different regions of an existing data set. The window, see figure 6, is divided into two parts. The upper part is a toolbar and the lower part is called working area in this manual.

Figure 5: A screenshot of the procedure for an EScan run. Note that a row is selected in the Parameter window.
Figure 6: The Data window with the toolbar, top, and the working area, the rest of the window.

**Toolbar**
The toolbar consists of four buttons and a drop-down choice list. The choice list is used to choose on which data set the operations should be conducted. The first button from the left loads data from a file to the active data set. The second button adds a new empty data set to the list. The third button deletes the active data set. The button furthest to the right plots the data in the main window.

**Working area**
The two upper input fields in the working area are labeled $x$ col, $y$ col and $e$ col\(^3\). The values in these fields represent which columns of the file contains the x data, y data and errors of the y data, respectively. This information is used when new data is loaded. The first column in the data file is denoted by 0. The text fields labeled $x=\$, $y=\$, and $error=\$ are used for writing Python expressions that operate on the raw data, as read from the file. By clicking on the Apply button the typed command is executed. At the end of this section some useful expressions are presented. There is a tick box labeled **use for fitting** at the bottom right of the window. If this box is checked the active data set will be plotted and used for fitting. At the bottom right there is another tick box that controls whether or not to plot the error bars of the data.

In this paragraph some useful expressions for treating the raw data are presented. Any Python expression will work and, in addition, if a special function is written in the model file this can be called to process the data. First of all to reset the data to the raw data write, $x$ in the x field and $y$ in the y field. The general syntax for selecting data from an array is $x[start:end:stride]$

If a special interval of the data needs to be fitted:

$x[20:-300]$

\(^3\)If no errors for the data are available set $e\, col=y\, col$
where the first value is the starting point (number of elements from the beginning) and the last is the end point. A negative value means that the end point is calculated from the end of the array. In addition, if the number of data points has to be decreased the expression above can be extended to include the stride.

\[ x[20:-300:2] \]

Consequently with this expression only every second data point is included. The operations shown here also need to be performed on the y values. This is done by typing the same expression into the text field for the y values and exchanging x against y. It is also possible to conduct simple arithmetic operations on the data. For example transforming the x data from degrees to \( Q_z \) (scattering vector in reciprocal Ångström), assuming that a wavelength of 1.54 Å is used:

\[ 4\pi/1.54\sin(x\pi/180) \]

This would then be typed into the text field for the x data. The examples presented here are rather limited but hopefully it shows the flexibility of treating the data. For a more detailed list of functions and syntax the reader is referred to the tutorials and manuals found at [www.scipy.org](http://www.scipy.org).

**Making a model**

As said before, the only mandatory thing the model file has to contain is a function called `Sim` taking a member of the class `Data` as input parameter. However, to make the model useful, functions for setting the values have to be incorporated. Since writing a model actually involves writing a script in Python it is good to have some basic knowledge of the syntax. However, if you have some basic knowledge about programming it should be fairly easy to just look at the examples and write your own models without having to learn to program in Python. On the other hand, there exists a number of free introductory books as well as tutorials on the internet for the interested reader, see below.

- Python’s homepage contain most of the available tutorials online, [www.python.org](http://www.python.org).
- *How to Think Like a Computer Scientist: Learning with Python* is a textbook for the beginner written for computer science students, [www.greenteapress.com/thinkpython](http://www.greenteapress.com/thinkpython).
- *Dive Into Python* is an introduction to Python for the more experienced programmer, [diveintopython.org](http://diveintopython.org).
- In addition there are a number of tutorials on the SciPy homepage, [www.scipy.org](http://www.scipy.org), which deal with numerical computations. There is also a migration guide for those who are familiar with MatLab®
In order to write the Sim class it is necessary to know the structure of the class Data which is taken as a parameter. The variables which could be useful in the Sim function are:

- **x** A list of 1-D arrays (vectors) containing the x-values of the processed data
- **y** A list of 1-D arrays (vectors) containing the y-values of the processed data
- **xraw** A list of 1-D arrays (vectors) containing the raw x-values (the data loaded from the data file)
- **yraw** A list of 1-D arrays (vectors) containing the raw y-values (the data loaded from the data file)
- **use** A list of booleans (True or False) denoting if the data should be fitted

Knowing what the Data class contains we will start with a simple example, making a model that fits one Gaussian to the first data set. The free parameters of the Gaussian are: the center of the peak, \( x_c \), the peak width, \( w \), and the amplitude of the peak, \( A \). Writing a model for it would produce a code as shown below. Note that a # produce a comment.

```python
# Init the variables
global w, xc, A
w=1.0
xc=0.0
A=1.0

# Define the function for a Gaussian
# i.e. definition of the model
def Gaussian(x):
    # Define the variables as global
global w, xc, A
    return A*exp((x-xc)**2/w**2)

# Define the functions for setting the parameters
# in the model
def setW(wtemp):
    global w
    w=wtemp

def setXc(xctemp):
    global xc
    xc=xctemp

def setA(Atemp):
    global A
```

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A=Atemp

# Define the function Sim
def Sim(data):
    # Calculate the Gaussian
    I=Gauss(data.x[0])
    # The returned value has to be a list
    return [I]

The following is a brief description of the code above. First the variables are initialized (created). The global keyword states that the variables are global and can be accessed from any function. After that a function for calculating a Gaussian variable is created, using the keyword global to make the parameters accessible. The function takes an array of x values as input parameters and returns the calculated y-values. Next the three functions for setting the parameters are defined. Each of them defines the variable as global before setting it to the value. These function names are the ones that should be put into the Parameters column of the spreadsheet in the parameter window. At last the Sim function is defined. The function Gauss is called to calculate the y-values with the x-data as the input argument. The x-values of the first data set are extracted as data.x[0], and those of the second data set would be extracted by data.x[1]. Note that a list is returned by taking the array (vector) I and making a list with one element. Note that this requires that only one data set has been loaded.

The code above is usually sufficient for prototyping and simple problems. For more complex models it is recommended to write a library. This is what has been done for the simulation of x-ray reflectivity data. Also, instead of writing a lot of functions for each model, a class, or several, can be written to make the model simple to use. As a more elaborate example the previous simple example can be transformed into a class:

# Definition of the class
class Gauss:
    # A class for a Gaussian
    # The creator of the class
    def __init__(self,w=1.0,xc=0.0,A=1.0):
        self.w=w
        self.xc=xc
        self.A=A

    # The set functions used in the
    # parameters column
    def setW(w):
        self.w=w
def setXc(xc):
    self.xc=xc

def setA(A):
    self.A=A

# The function to calculate the model
# (A Gaussian)
def Simulate(x):
    return A*exp((x-self.xc)**2/self.w**2)

# Make a Gaussian:
Peak1=Gauss(w=2.0,xc=1.5,A=2.0)

def Sim(data):
    # Calculate the Gaussian
    I=Peak1.Simulate(data.x[0])
    # The returned value has to be a list
    return [I]

This code is quite similar to the first version with only functions. It starts with the definition of the class Gauss. This class has a constructor, __init__, to initialize the parameters of the object and functions to set the member variables, denoted as self.*. It also contains a member function to calculate a Gaussian with the member variables. After the class definition an object, Peak1, of the Gauss class is created. Then the Sim function is defined as in the previous example but with the function call exchanged to Peak1.Simulate(data.x[0]) in order to simulate the object Peak1. The function names that should go into the parameter column in the parameter window will be: Peak1.setW, Peak1.setXc and Peak1.setA. Making the model based on a class makes it easier to extend. For example if two peaks should be fitted the class does not have to be changed. Instead an additional object of the class Gauss, for example called Peak2, can be created and the two contributions are then added in the Sim function. The code would then be modified to (omitting the class definition):

#Insert the class definition from above
# Make Gaussians:
Peak1=Gauss(w=2.0,xc=1.5,A=2.0)
Peak2=Gauss(w=2.0,xc=1.5,A=2.0)

def Sim(data):
    # Calculate the Gaussian
Thus, for fitting the parameters for the second Gaussian the functions used should be Peak2.setW, Peak2.setXc and Peak2.setA. When the base class is created it can be extended with more problem oriented constraints by using functions as in the first example. For example, in some cases it might be known that the width of the two Gaussians should be the same. This can be solved by defining a new function:

```python
# Insert the class definition from above
# Make a Gaussians:
Peak1=Gauss(w=2.0, xc=1.5, A=2.0)
Peak2=Gauss(w=2.0, xc=1.5, A=2.0)

def setBothW(w):
    Peak1.setW(w)
    Peak2.setW(w)

def Sim(data):
    # Calculate the Gaussian
    I=Peak1.Simulate(data.x[0])
    +Peak2.Simulate(data.x[0])
    # The returned value has to be a list
    return [I]
```

Instead of using the *.setW functions the setBothW can be used. In summary it is recommended that the models implemented in libraries are defined as classes and that these are as general as possible with respect to the parameters. The specific parameter couplings can be included as functions in the model file. The methods shown with the examples in this section also apply to the libraries included for x-ray reflectivity. The classes are different but the general use is the same.

The figure of merit function

The figure of merit (FOM) function is the function that describes how good the model fits with the data. In the program the error functions can be defined as a function in the model file or by using a predefined FOM function in the file errorfuncs.py. All the error functions defined below are implemented in this file.

In most cases of fitting, for example a straight line, the method of least squares is usually used. This is a special case of the more general Chi-squared,
\[ \chi^2, \text{method.} \]

\[ \chi^2 = \text{FOM}_{\text{Chi2Bars}} = \sum_i \left( \frac{M_i - S_i}{\sigma_i} \right)^2, \]  

(7.1)

where \( M_i \) represents the measured value, \( S_i \) the simulated value and \( \sigma_i \) is the error. The index \( i \) represents the \( i \)'th point. This should be considered as the starting point for any fitting problem. If error bars are not available for the data or if the data has large systematic errors one can consider the functions below instead. A useful FOM function for reflectivity and diffraction is the absolute logarithmic difference;

\[ \text{FOM}_{\text{log}} = \frac{1}{N-1} \sum_i |\log(M_i) - \log(S_i)|, \]  

(7.2)

where \( N \) is the number of points. This normalization with the number of points is included in order to compare different data sets. Otherwise the error function would be dependent on the number of points to be fitted. A similar FOM function is the squared logarithmic

\[ \text{FOM}_{\text{log}} = \frac{1}{N-1} \sum_i (\log(M_i) - \log(S_i))^2, \]  

(7.3)

which is more sensitive to outlying data points than the previous, due to that the error is squared. Thus it is usually not as useful as the absolute logarithmic error function. Another FOM function that has been found useful for high angle diffraction from superlattices is the absolute squareroot

\[ \text{FOM}_{\text{sqr}} = \frac{1}{N-1} \sum_i \left| \sqrt{M_i} - \sqrt{S_i} \right|, \]  

(7.4)

This will put more emphasis on the points of high intensity than \( \text{FOM}_{\text{log}} \) and can be more useful in those cases where the intensity range is not too large or where the features that should be fitted have high intensity.

The default FOM function in the program is the absolute logarithmic error function. To change the error function used, append the following line to the model file, using the FOM function called \texttt{MyFom}.

\begin{verbatim}
    solver.setFomfunc(\texttt{MyFom})
\end{verbatim}

For the names of the other FOM functions open the file \texttt{fomfuncs.py}. It is also possible to add a user defined FOM function in the model file. The syntax for writing an error function is

\begin{verbatim}
def NameFom(data,sim):
    return 1/sum(data.use)*sum([expression for
                (y,s,use) in zip(data.y,sim,data.use)
                if use])
\end{verbatim}

The \texttt{for} loop is necessary since there can be more than one data set that is used in the fitting procedure. \texttt{expression} should be replaced with the expression for the new error function.
Libraries

This section will give an introduction to the model included in the program. Also some examples on how to write the model will be given. If the first section is unclear, read the section Making a Model again since the same syntax is used in that section. The examples are also less complex.

X-ray reflectivity

The libraries for x-ray reflectivity are built from the concept of three building blocks for a sample. These are: Layer, Stack and Sample. The Layer defines the parameters of a layer (e.g. refractive index, roughness). The Stack contains a number of Layers which can be repeated a number of times. This corresponds in some way to a multilayer. The Sample contains a number of stacks which builds up the sample. Also included is the ambient medium as well as the substrate. A picture of how the different classes make up a sample can be seen in figure 7. A class named Instrument is also included for various instrument parameters (e.g. wavelength).

Usage

In order to use a model library it should be imported into the model file by the import statement. The current model for x-ray reflectivity is called ModelInterdiff. As an example consider the sample consisting of a Fe/Pt multilayer with 25 repeats on top of a buffer layer that consists of a Fe layer closest to the substrate and then a thick Pt layer. The sample has been grown on MgO. In order to model this sample two different stacks are needed: one
for the buffer layers and the second for the multilayer. The model file would look something like the following.

```python
# Import the model classes
from ModelInterdiff import *

# get the refractive indexes for the materials
nFe=getn('Fe1',2/2.866**3,1.54)
nPt=getn('Pt1',4/3.924**3,1.54)
nMgO=getn('Mg1O1',4*2/4.2**3,1.54)

# Create all the layers needed
MLFe=Layer(n=nFe,d=13.5,sigmar=1.0,reldens=1.0)
MLPt=Layer(n=nPt,d=13.5,sigmar=1.0,reldens=1.0)
bufPt=Layer(n=nPt,d=40,sigmar=1.0,reldens=1.0)
bufFe=Layer(n=nFe,d=5,sigmar=1.0,reldens=1.0)
sub=Layer(n=nMgO,sigmar=5,reldens=1.0)

# Create the Stacks - consists of layers
ML=Stack(Layers=[MLFe,MLPt],Repetitions=25)
buf=Stack(Layers=[bufFe,bufPt],Repetitions=1)

# Create the sample
sample=Sample(Stacks=[buf,ML],Ambient=Layer(n=1.0),Substrate=sub)

# Create the instrument -
# Coordinates=1 => two theta Coordintes =0 => Q_Z
inst=Instrument(Wavelength=1.54,Coordinates=1,I0=1.0e6)

# Simulate function - MANDATORY
def Sim(data):
    I=sample.SimSpecular(data.x[0],inst)
    return [I]
```

First the script imports the library `ModelInterdiff`. This loads the underlying model. Next the different refractive indices for the materials are extracted from the scattering length tables[94]. The function `getn` takes the atomic composition of the elements as a string as first argument, the second argument is the atomic density in atoms/Å³ and the the last argument is the x-ray wavelength in Å. In the next code block all the layers needed are created. The constructor for the `Layer` class takes the following parameters as input:
1. `n`, the refractive index of the material.
2. \( d \), the thickness of the layer in Å.
3. \( \text{sigmar} \), the roughness of the upper interface in Å.
4. \( \text{reldens} \), the relative density of the material, where 1.0 corresponds to the (bulk)density that \( n \) refers to.

After the layers have been created the different stacks are created, one for the multilayer and one for the buffer layers. The constructor for a \texttt{Stack} takes the layers that are contained in that stack as a list and the number of repeats of that stack. Note that the first layer in the list is the layer closest to the substrate. When the stacks have been created the sample can be constructed from these stacks. The constructor for a \texttt{Sample} takes three input parameters: a list of the Stacks, the Ambient layer (what is on top of the multilayer, usually air, \( n = 1 \)) and the substrate layer. For the ambient layer the calculations ignore the roughness and the thickness. For the substrate the calculations ignore the thickness. The first element in the \texttt{Stacks} list is the one closest to the substrate.

Next an \texttt{Instrument} object is created. This contains the wavelength used and in which coordinates the data was recorded; 1 corresponds to \( 2\theta \) and 0 corresponds to \( Q_z \). In addition it contains the incident intensity \( I_0 \). Finally the \texttt{Sim} function is created. The function \texttt{sample.SimSpecular} calculates the specular reflectivity from the sample given the x-data and the instrument object.

In order to use the model file for fitting all the functions for setting the parameters have to be known. These functions are named according to the following rule: \texttt{Objectname.set[parameter name-first letter uppercase]}. For example, to fit all the parameters for the object \texttt{MLFe} the functions would become: \texttt{MLFe.setD}, \texttt{MLFe.setN}, \texttt{MLFe.setSigmar} and \texttt{MLFe.setReledens}. Note that it is not recommended to fit \( n \) since this is a complex number and the fitting program only works with real numbers.

The model \texttt{ModelInterdiff} also contains a function to calculate the diffuse reflectivity from a multilayer stack, \texttt{[sample].SimOffSpecular(TwoThetaQz,ThetaQx,inst)}. To simulate diffuse reflectivity some more parameters has to be defined for the sample, \texttt{eta_x} the in-plane correlation length in Å, \texttt{eta_z} the out-of-plane correlation length between the interfaces and \texttt{h} the jaggedness parameter. Note that these parameters are assumed to be constant throughout the sample. In addition, the amount of interdiffusion of each layer can be defined as \texttt{sigmai}.

**Description**

This section will give an introduction to the different files and functions for the classes used for simulating the reflectivity. This could become a bit confusing for the reader not familiar with programming. It is mainly intended for people wanting to extend the models while keeping the general interface the same.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>n</td>
<td>A complex number for the refractive index of the layer. It should be on the form $n = 1 - \delta + \beta j$</td>
</tr>
<tr>
<td>d</td>
<td>The thickness of the layer given in Å.</td>
</tr>
<tr>
<td>sigmar</td>
<td>The root mean square (rms) value of the roughness given in Å.</td>
</tr>
<tr>
<td>sigmai</td>
<td>The root mean square (rms) value of the interdiffusion given in Å. Note that the roughness used for specular calculations is $\sigma = \sqrt{\sigma_i^2 + \sigma_r^2}$.</td>
</tr>
<tr>
<td>reldens</td>
<td>The relative density of the material. Used as a scaling factor for $\delta$ and $\beta$ in the refractive index.</td>
</tr>
</tbody>
</table>

Table 7.1: The different parameters for the class Layer.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Layers</td>
<td>A list of the different Layers in the Stack. Thus the input should be on the form $\text{Layers}=[\text{layer1,layer2}]$</td>
</tr>
<tr>
<td>Repetitions</td>
<td>The number of times the stack repeats itself. Should be an integer.</td>
</tr>
</tbody>
</table>

Table 7.2: The different parameters for the class Stack.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stacks</td>
<td>A list of the different Stacks in the Sample. Thus the input should be on the form $\text{Stacks}=[\text{stack1,stack2}]$.</td>
</tr>
<tr>
<td>Ambient</td>
<td>The Ambient layer, i.e. material that is on top of the sample. Should be a member of the class Layer.</td>
</tr>
<tr>
<td>Substrate</td>
<td>The Substrate layer, i.e. material that is below the sample structure. Should be a member of the class Layer.</td>
</tr>
<tr>
<td>h</td>
<td>The jaggedness parameter. Only used for diffuse calculations. Should be in the interval $[0.15, 1.0]$.</td>
</tr>
<tr>
<td>eta_z</td>
<td>The out-of-plane correlation length given in Å.</td>
</tr>
<tr>
<td>eta_x</td>
<td>The in-plane correlation length given in Å.</td>
</tr>
</tbody>
</table>

Table 7.3: The different parameters for the class Sample.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength</td>
<td>The wavelength of the radiation used given in Å.</td>
</tr>
<tr>
<td>Coordinates</td>
<td>The coordinates which the data are in. Has to be an integer. 0 corresponds to reciprocal coordinates in Å$^{-1}$ and 1 to angular coordinates, i.e. the scattering angle, 2(\theta) in degrees.</td>
</tr>
<tr>
<td>I0</td>
<td>The incident intensity. A scaling factor for the reflectivity.</td>
</tr>
<tr>
<td>Restype</td>
<td>An integer determining which type of resolution convolution to do. 0 no resolution convolution. 1 fast convolution assuming equally spaced data points with a spacing much smaller than the resolution and Gaussian distribution. 2 &quot;Full convolution&quot; calculates Respoints data extra and convolutes these with a Gaussian.</td>
</tr>
<tr>
<td>Res</td>
<td>The resolution of the instrument, given as a standard deviation in the same units as the data.</td>
</tr>
<tr>
<td>Respoints</td>
<td>The number of points used for the resolution convolution. Only valid for Restype=2</td>
</tr>
<tr>
<td>Resrange</td>
<td>How many standard deviations given by Res that are included in the convolution.</td>
</tr>
<tr>
<td>Footype</td>
<td>An integer determining which footprint correction to use. 0: no footprint correction. 1: footprint correction for a gaussian beamprofile. 2: footprint correction for a square beamprofile.</td>
</tr>
<tr>
<td>Beaw</td>
<td>The width of the beam at the sample position given in mm. For Footype=1 it is the rms width of the beam. For Footype=2 it is the FWHM of the beam. Used for footprint corrections.</td>
</tr>
<tr>
<td>Samlen</td>
<td>The sample length given in mm. Used for footprint corrections.</td>
</tr>
</tbody>
</table>

Table 7.4: The different parameters for the class Instrument.
The underlying calculation routine is implemented in the file `Paratt.py` where the function `Refl` is implemented. This function takes the refractive indices, thicknesses and roughnesses of the layers as 1-D arrays. Thus it does not make use of the classes defined in the previous section. In order to make the implementation of a new model as easy as possible the classes are created dynamically with the `MakeClasses` function in the file `Refl.py`. This function takes a dictionary that contains the parameter names and their default values as input parameters. The function then returns the classes. This function allows easy creation of the interface of any model based on the Layers-Stacks-Sample concept. As an example how to tie these two libraries together see the file `ModelInterdiff.py`. This file defines the model and extracts the parameters from the classes and sends them to the `Refl` function for calculation. The definition of the classes in `MakeClasses` utilizes metaclasses to create all the parameter functions and the parameters dynamically. The process of creating the classes provides a very flexible framework for creating new models.

The fitting algorithm

A general introduction to differential evolution can be found at [31]. For the specific case of the application of the algorithm to x-ray reflectivity and diffraction the reader is referred to the paper of Wormington et al.[32].

This section will briefly deal with the parameters the user can change to tune the algorithm. However, this should not be necessary for most problems, the algorithm usually works as it is. The class that implements the differential evolution algorithm is called `Solver` and can be found in the file `DEWorm.py`. In the program an instance of this class is created and called `solver`. The parameters that could be useful to change are:

- **km** The mutation constant. The default value is 0.7. A reasonable value is usually between 0.5 and 1. A lower value yields a faster convergence but also a higher probability of misconvergence. Example: `solver.setKm(0.7)`

- **kr** The crossover constant. Default value is 0.5. Determines the probability that a parameter in the present vector is exchanged. Should be between 0 and 1. Example: `solver.setKr(0.5)`

- **Popmult** A multiplicative factor that determines the size of the population. The population size is determined by Popmult×The number of free parameters. The default value is 3. Example: `solver.setPopmult(3)`

- **maxGenMult** A multiplicative factor that determines the maximum number of generations/iterations. The maximum number of generations
is determined by the number of free parameters \( \times \) population size \( \times \) maxGenMult. The default value is 1. Example: 
\[
solver.setMaxgenmult(1)
\]

**FOMFunc** The function that calculates the error. See the section 7 for more details. Example: 
\[
solver.setFomfunc(Chi2Fom)
\]

Note that the initial parameter settings for the fitting algorithm are optimized for many free parameters. Fitting only one parameter will not work properly. The minimum number of free parameters for these settings are about 3-4 free parameters in order to get reasonable results.

**A short HowTo for x-ray reflectivity**

1. Get the x-ray data, do not use too fine steps since this will increase the computation time. Check if the sample is bent or “wavy”. If that is the case try to decrease the resolution. In case of reflectivity data check that the diffuse scattering does not contribute to the specular intensity. If so, subtract it.
2. Write a model file, using your knowledge of the system. Make the Sim function. Couple parameters to make them more independent. For example, use the bilayer repetition length as a free parameter for multilayers. Do not forget to reload the model file when it has changed.
3. When the model file works include the instrument resolution (convolution with a Gaussian is often good)[95–98]. If needed, include the footprint correction[98].
4. Remember to choose an error function that makes sense for your problem. This is an important point.
5. Cut out the region that does not contain any information, mainly for speeding up the calculation.
6. Define all free variables in the grid/spreadsheet.
7. Type in reasonable minimum and maximum values. Be generous with the bounds.
8. Set a start guess. A rough guess is enough.
9. Start fitting. Keep an eye on the parameter distribution; if the population spread (blue bars) is very small there will be very little improvement.
10. If the best value converges to the min or max boundaries increase the min and max values. Restart the fit.
11. If the fit is not good enough there are three possibilities:
   - Check the data. Make sure that the sample is not for example bent (varying width of the specular component). This is best checked at a couple of angles close to the total reflection and also far away.
   - The model is wrong - change it to a better one.
• The error function does not give a good representation of the features you want to fit.

12. Fix the problem mentioned previously and restart the fitting process.
13. Continue until the fit is good (repeat 9-12).
Swedish Summary

En strukturell synvinkel på magnetism i Fe- och Co-baserade supergitter

Magnetismforskningen har under de senaste årtiondena skiftat sitt fokus från undersökning av bulkegenskaperna4 till att studera ytegenskaperna hos materialen. Vid ytor har atomerna en annan omgivning och de fysikaliska egenskaperna hos materialen ändras. Följaktligen kan materialens egenskaper ändras kraftigt om ytan modifieras eller om material med stor andel ytor tillverkas. Dessa material kan syntetiseras antingen som tunna filer eller som partiklar. Eftersom den del av materialet som påverkas av ytan vanligtvis är väldigt liten, typiskt ett par atomer tunn, måste tillverkningen av dessa material ske med atomär precision. Den här grenen av magnetismforskningen utvecklades naturligt när den nödvändiga teknologin fanns tillgänglig för att kunna tillverka material syntetiskt på atomär skala. Samtidigt som forskningen är en drivkraft i sig själv finns det ett stort intresse från industrin eftersom de nya materialen kan ge bättre produkter. Det kanske mest slående exemplet är hårddiskar vilka har fått en stor ökning i kapacitet som en direkt följd av forskning inom magnetism. En stor del av kapacitetsökningen hos hårddiskar började på 1980-talet då den gigantiska magnetoresistanseffekten (GMR) upptäcktes. Sensorer baserade på denna effekt implementerades snabbt i läshuvudet på hårddiskarna. I dag fokuserar forskningen mer på själva lagringsmediet, som behöver förbättras avsevärt för att kunna innehålla mer information per ytenhet. Den största utmaningen är att hitta material som kan lagra stora mängder information och samtidigt vara stabila under lång tid. Detta kräver material som har stark magnetokristallin anisotropi, läsning av den magnetiska riktningen, för att undvika utradering av informationen på grund av termiska fluktuationer (värmerörelser). Men om materialen har stark magnetokristallin anisotropi blir det svåra att skriva och ändra information, och därför behöver materialet vara starkt magnetiskt, d.v.s. ha ett högt magnetiskt moment. En del av arbetet bakom denna avhandling består av syntetisering och karakterisering av ett material bestående av en (Fe,Co)-legering som har föreslagits utifrån teoretiska beräkningar och som skulle kunna vara ett lämpligt material för framtidens hårddiskar.

4 ‘De egenskaper hos materien i en kropp som är relaterade till kroppens hela volym. De är i motsats till ytegenskaper inte beroende av ytans tillstånd.’ (Nationalencyklopedin)
Figur 1: En bild av ett idealt enkristallint multilager. De tjocka (ljusare) linjerna markerar den minsta repeterande enheten hos respektive material, en så kallad enhetscell.

Arbetet presenterat i denna avhandling består av undersökningar av de magnetiska egenskaperna hos tunna filmer, i synnerhet vid gränssytorna till andra material. Eftersom gränssytorna består av väldigt lite material är det fördelaktigt att producera prover som innehåller många gränssytor i stället för bara en. Detta görs genom att repetera de gränssytor man vill undersöka ett antal gånger. En sådan struktur kallas för ett multilager och kan ses i figur 1. För att de fundamentala magnetiska egenskaperna ska kunna förstås är det viktigt att växa proverna under mycket ren förhållanden så att föroreningar undviks. De prover som studerats är växta med hjälp av sputtring av högrena material under ultrahögvakuumlika omständigheter. Det betyder att trycket i tillväxtkammaren är ungefär 1 biljondel (10^{-12}) av det normala lufttrycket. Ytterligare en viktig detalj är att proverna bör växa så att de består av bara en kristall, så att riktningarna i materialet är väldefinierade relativt atomstrukturen. Detta gör att de största defekterna i materialen, nämligen korngränser mellan perfekta områden, undviks. Hur atomerna i ett sådant idealt prov kan vara ordnade visas i förstoringen i figur 1. Tyvärr är det i verkligheten nästan omöjligt att växa ett prov som det i figuren. Eftersom tillväxten inte är ideal kommer det alltid att uppstå ojämnheter i skiktjockleken. Vissa materialkombinationer kan också blanda sig med varandra vid gränssytorna. Slutligen kan det också uppstå kristallina defekter, som dislokationer, på grund av spänningar mellan de olika materialen i provet. Eftersom det är omöjligt att uppnå fullständig perfektion i materialen måste de ovan nämnda defekterna noggrant karakteriseras. Ett sätt att göra detta är att använda t.ex. röntgendiffraktion. Röntgenstrålning har en våglängd av samma storleksordning som atomernas inbördes avstånd, och därför uppstår ett interferensmönster som berättar om strukturen och defekterna hos materialet. Modeller kan sedan anpassas till diffractionsmönstret för att utvinna strukturinformation. En del av arbetet har bestått i att utveckla da-
torprogram och modeller för strukturbestämningen av multilager. Den metod som har använts mest för att bestämma de magnetiska momenten för materi-alen i denna avhandlingen kallas röntgenbaserad magnetisk cirkulär dikroism (X-ray Magnetic Circular Dichroism, XMCD). XMCD använder absorption av röntgenljus för att bestämma det magnetiska momentet hos atomer, till skillnad från de flesta andra metoder som direkt mäter det sammanlagda magnetiska momentet från hela provet. Fördelen med XMCD jämfört med andra metoder är att det magnetiska momentet hos olika grundämnen kan särskiljas. För att kunna använda XMCD krävs tillgång till en synkrotronljuskälla, och vi har använt Sveriges synkrotronanläggning, MAX-lab, i Lund.

De arbeten som presenteras i denna avhandling visar på vikten av att pre-cist kunna karakterisera de strukturella egenskaperna hos multilager och lik-nande material. Detta är avgörande för att vi ska kunna förstå det magnetiska beteendet hos materialen. Dessutom är det av stor vikt när de teoretiska beräkningarna av vanligtvis perfekta material ska jämföras med de material som tillverkas.

Multilager av Fe och Co studerades eftersom tidigare undersökningar hade antytt att det magnetiska momentet i dessa strukturer kunde ha ett totalt mag-netiskt moment högre än det man kunde finna i legeringen. Det bör sägas att en speciell legering av Fe och Co (ca 30% Co) erhåller det högsta magnetiska momentet bland alla existerande material. De senaste resultaten visade dock att det totala magnetiska momentet inte blev högre i dessa strukturer. Det magnetiska momentet för Fe-atomerna nådde vid gränsytorna samma värde som det för Fe-atomer i legeringen. Co-atomernas magnetiska moment var konstant för de prover som studerades.

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