Magnetism and Structure in Metallic Multilayers

BY

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Abstract


The interplay between magnetism and structure has been studied in magnetic multilayers by electronic structure calculations based on density functional theory and analyzed in terms of models. The main ideas behind the Korringa-Kohn-Rostocker Green’s function method are described and the implementation of the coherent potential approximation is outlined.

A simple model for the bilinear magnetic interlayer coupling in metallic multilayers is derived that elucidates the main characteristics of the effect such as coupling period and origin of damping. An analysis of two exotic effects on the magnetic interlayer coupling, Fermi surface nesting and magnetic enhancement is also performed. The Fermi surface nesting in CuPd for the (110) direction is shown to induce a sharp peak in the magnetic interlayer coupling amplitude for a Fe/CuPd/Fe system when the Cu concentration is 60% in the CuPd alloy. The high magnetic susceptibility in Pd is shown to have strong influence on the magnetic interlayer coupling in a Fe/Pd/Fe (100) system where it changes the amplitude, phase and induces an offset.

The relation between surface structure and magnetic properties in metallic multilayers is investigated in terms of a theory that is based on a symbiosis between experiment and theory. By calculating the total magnetic moment of a sample for a large range of possible interface structures and comparing to experimental results for equivalent samples a parameter that describes the interface structure is determined. This parameter is then shown to be universal for the particular combination of elements in the structure both as regards the calculated total magnetic moment as well as the magnetic interlayer coupling and the critical temperatures.

Keywords: Magnetism, Interfaces, Structure, KKR-ASA, CPA, Quantum Well

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To Bandilita
List of papers

This thesis is based on the collection of papers given below. Each article will be referred to by its Roman numeral.

I Giant magnetic enhancement in Fe/Pd films and its influence on the magnetic interlayer coupling
E. Holmström, L. Nordström and A. M. N. Niklasson

II The Fermi surface effect on magnetic interlayer coupling
E. Holmström, A. Bergman, L. Nordström, I. Abrikosov, S.B. Dugdale and B.L. Györfy
In manuscript.

III On the interface structure of metallic multilayers
E. Holmström, L. Bergqvist, B. Skubic, B. Hjörvarsson, L. Nordström, I. Abrikosov and O. Eriksson
In manuscript.

IV Magnetic moments and exchange interactions in FeNi/V multilayers
B. Skubic, E. Holmström, O. Eriksson, A. M. Blixt, G. A. Andersson, B. Hjörvarsson and V. Stanciu
In manuscript.

V Magnetic phase diagram of Fe$_{0.82}$Ni$_{0.18}$/V(001) superlattices
A. M. Blixt, G. Andersson, V. Stanciu, B. Skubic, E. Holmström, P. Nordblad and B. Hjörvarsson
In manuscript.

VI Alloying as a method of tuning the interlayer exchange coupling in Fe/V multilayers
B. Skubic, E. Holmström, O. Bengone and O. Eriksson
_In manuscript._

VII **Theory of spin filtering through quantum dots**
J. Fransson, E. Holmström, O. Eriksson and I. Sandalov

VIII **Influence of interface mixing on the magnetic properties of BCC Fe$_{0.82}$Ni$_{0.18}$/V (0 0 1) superlattices**
G. Andersson, A.M. Blixt, V. Stanciu, B. Skubic, E. Holmström and P. Nordblad

IX **Geometric and electronic structure of PdMn bimetallic systems on Pd(100)**
A. Sandell, P. H. Andersson, E. Holmström, A. J. Jaworowski, and L. Nordström

X **Observation of short- and long-range hybridization of a buried Cu monolayer in Ni**

XI **Probing surface states of Cu/Ni thin films using x-ray absorption spectroscopy**

XII **The stability of metallic vicinal surfaces: Application of an _ab-initio_ order-N method**
S. Shallcross, E. Holmström
_In manuscript._

XIII **Core-level shifts for surface bimetallic systems from first-principles theory: Pd-Mn structures on Pd(100)**
W. Olovsson, E. Holmström, A. Sandell, and I. A. Abrikosov
XIV Magnetism of Fe/V and Fe/Co multilayers
O. Eriksson, L. Bergqvist, E. Holmström, A. Bergman, O. LeBacq,
S. Frota-Pessoa, B. Hjörvarsson and L. Nordström

XV Structural and magnetic aspects of multilayer interfaces
E. Holmström, L. Bergqvist, B. Skubic and O. Eriksson

XVI Local and global magnetism in random FeV alloys
E. Holmström, R. Lizárraga, S. Shallcross and I. A. Abrikosov
In manuscript.

XVII Magnetocrystalline anisotropy of decorated and undecorated steps
of the (11n) Co vicinals
S. Shallcross and E. Holmström
In manuscript.

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Comments on my contribution
In the papers where I am the first author I am responsible for the main part of
the work, from ideas to the finished papers. Concerning the other papers I have
contributed in different ways, such as ideas, various parts of the calculations,
development of computational tools and participation in the analysis.
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Chapter 1

Introduction

On the front page of this thesis is a map. A map is a reduced picture of the landscape that is simplified by using special symbols. Most people can understand a map since it describes things that we are very used to from our everyday lives such as mountains, lakes and roads. The concept of a map has many similarities to the language of science since the goal in science is also to describe reality by using a symbolic language. In this case it is called mathematics and is much more complex in its structure than the symbols that are used on maps.

The mathematical equations that are used in science may be quite well known or they may be of such a nature that the people in the research frontier just have a vague hunch of their actual form. In any case there is always a limit of the known and the actual position of this limit is just dependent of how complex phenomena that are studied. For example, it is very well known that Newton's second law should describe the motion of the planets to a very high accuracy, but the question of how all individual stars in the galaxy will move is such a complex problem that the exact answer is unknown. On the other hand there are branches of theoretical physics that try to unify all known physical theories in one single unifying theory where very little is known about the basic equations.

A map is very useful when you want to know where you are and put yourself into perspective and in figure 1.1 a map is displayed that tries to show some different branches of science and their position in the landscape of equation uncertainty and complexity. This thesis is in condensed matter physics and this branch is positioned at a place where the basic underlying equations that describe the phenomena are fairly well known so the complexity of the problems that can be investigated is quite high. The development of modern computers and very efficient theories have made it possible to investigate these complex systems and consequently, all results in this thesis are based on large computer calculations.
Chapter 1. Introduction

Complexity of phenomena
Uncertainty about basic equations

known

Meterology Turbulence
Condenced matter physics

Quantum gravity
Particle physics
Chemical reactions

UNKNOWN

Social science
Living systems
Economics
Climate

Figure 1.1: A schematic map that tries to describe the degree of uncertainty that exists in the underlying mathematical expressions describing different phenomena as a function of the complexity of the phenomena. The borderline between the KNOWN and UNKNOWN may not actually be smooth and there should probably be areas of KNOWN in the UNKNOWN as well as UNKNOWN in the KNOWN. Freely interpreted after illustration in ref.1

This thesis is based on the manuscripts and published articles that are included in the end of this book. The first part is meant as an introduction to the particular part of the field of magnetic multilayer physics that was investigated in the articles. By discussing various simple models and concepts the introduction is hopefully useful as a starting point for further studies.
The theoretical methods

2.1 Introduction

A basic principle of nature is that the laws of physics do not change with time and a striking consequence from this fact is the conservation of energy for an isolated system. This means that energy can never be destroyed but only transformed into new forms. If we consider a system that is in weak contact with the surrounding it can be shown that the small disturbance from the outside will introduce finite lifetimes for all excited states. In fact, the disturbance may be as small as the interaction with the fluctuations of the vacuum itself. This means that every system that we want to describe will interact with the surrounding and evolve toward the lowest energy state (ground state). In reality, no solid is ever in the ground state because of the input of energy, for example by radiation, but for many practical purposes the ground state does give a very good description of the properties of the material.

The Schrödinger equation

The quantum mechanical way to calculate the properties of a system is to solve the Schrödinger equation. The time independent Schrödinger equation is generally written as

\[ \hat{H}\Psi = \varepsilon \Psi \]  

(2.1)

where \( \hat{H} \) is an object that contains the complete information about all interactions in the system that the equation describes. It is referred to as the Hamiltonian operator that acts on the object \( \Psi \). A bit handwaving, \( \Psi \) can be described as something that tells you about the current state of the system. It is therefore called the state vector or the wave function depending on how it is treated mathematically. \( \varepsilon \) is finally the total energy for the system in the particular state \( \Psi \). This equation is a very general formulation that sets out to describe...
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everything about the system that is investigated. The ground state energy of the system is then the solution of the Schrödinger equation that has the lowest energy.

Density functional theory

The problem with the Schrödinger equation is that it is possible to write down for most systems but never possible to solve exactly, except in some very few cases. The reason is the extreme complexity that the Hamiltonian takes for systems consisting of three particles or more, and a solid consists of typically $10^{23}$ atoms! If we only consider the electrons in the solid \( \Psi \) must at least contain the coordinates of all electrons in order to represent the state of the system. Actually this seems to be an impossible problem already when there are three particles involved. The natural question is then: How to find the total energy \( E \) of a solid when nobody can solve the Schrödinger equation for more than 2 particles? A route to solve the problem was presented by Hohenberg and Kohn\(^3\) by the development of the density functional theory (DFT) for electron systems and in 1998 Walter Kohn was rewarded the Nobel prize for his development of this theory.

In DFT the central quantity is not the wave function but the electron density \( n(r) \) that can be calculated as

\[
n(r) = \int d^3r \sum_{i=1}^{N} |\Psi(r_1, r_2, ..., r_N)|^2 \delta(r - r_i), \tag{2.2}
\]

if the wavefunction of the whole system is known, that is if we already have the solution to the Schrödinger equation. The theorems that Hohenberg and Kohn stated show that under very general conditions the electron density and the potential that the electrons experience are determined by each other and that there is a functional \( E[n(r)] \) that is minimized by the ground state electron density.

If the functional \( E[n(r)] \) could be found and minimized, there is a possibility to calculate the ground state total energy from the electron density alone. This is a fantastic simplification of the very difficult problem that the Schrödinger equation represents since the density is a single valued function that only depends on the position in space whereas the wavefunction is at least a function of all coordinates of all interacting electrons in the system.

The Kohn-Sham equation

Even with the reduced complexity of the problem that the DFT gives us, we are still faced with the difficulty of calculating the electron density \( n(r) \) (without knowing \( \Psi \)) and finding the functional \( E[n(r)] \). The functional for the total energy is of course still extremely difficult to find exactly. It would include
all physics of the system, including the effects that can only be described by collective behavior of electrons, the so called many-body effects. Examples of many-body effects are superconductivity (at least two electrons are needed to form a Cooper pair), itinerant magnetism (all electrons with one spin are shifted in energy with respect to the other spin) and the core level shift (the change in energy by exciting a core electron to the valence band depends on the amount of screening from all other electrons). Kohn and Sham\(^4\) showed that the functional \(E[n(r)]\) can be decomposed as

\[
E[n(r)] = \int V_{\text{ext}}(r)n(r)\,dr + \frac{1}{2} \int \int \frac{n(r)n(r')}{|r-r'|}\,dr\,dr' + T_s[n(r)] + E_{xc}[n(r)] 
\]  

(2.3)

where the terms are the potential energy from the nuclei, the Coulomb energy, the kinetic energy of a non-interacting electron gas and the exchange-correlation energy respectively. The non-interacting electrons, or quasiparticles, that were introduced then obeys the one particle Schrödinger equation

\[
\left\{ -\frac{1}{2} \nabla^2 + V_{\text{eff}}[n(r)] \right\} \psi_i(r) = \epsilon_i \psi_i(r)  
\]  

(2.4)

where \(V_{\text{eff}}[n(r)]\) is an effective potential that the electrons feel and \(\psi_i(r)\) is the wave function for the non-interacting electrons. The effective potential that was introduced was derived by Kohn and Sham to be

\[
V_{\text{eff}}[n(r)] = V_{\text{ext}} + \int \frac{2n(r')}{|r-r'|}\,dr' + \frac{\delta(n(r)\,E_{xc}[n(r)])}{\delta n(r)}.  
\]  

(2.5)

The density may then easily be calculated by a sum of the one particle densities as

\[
n(r) = \sum_{i=1}^{N} |\psi_i(r)|^2.  
\]  

(2.6)

The beauty of this approach by Kohn and Sham is that the complex many-body problem that the Schrödinger equation presents is transformed into a one particle problem that, when solved, will produce the correct electron density. The equations 2.4 to 2.5 have to be solved self-consistently by starting from an approximate atomic density, usually obtained by overlapping atomic densities and the resulting stationary self-consistent density can then be used in eq 2.3 to find the corresponding energy.
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\[ H_{\text{eff}} \psi_i = \epsilon_i \psi_i \]
\[ n(r) = \sum |\psi_i|^2 \]
\[ V_{\text{eff}}(n(r)) = V_{\text{ext}} + \int \frac{2n(r')}{|r - r'|} dr' + \frac{\delta(n(r)\xi_{xc}[n(r)])}{\delta n(r)} \]

Figure 2.1: The flow chart for a self-consistent solution of the Kohn-Sham equation. The self-consistently calculated electron density is then used in eq. 2.3 in order to obtain the total energy.

2.2 The KKR-ASA Green’s function method

In order to solve the Kohn-Sham equation efficiently on a computer it is necessary to describe the wavefunctions in a basis. To make the calculation as accurate and fast as possible, a small basis set is needed. In most schemes, such as the Korringa-Kohn-Rostocker method and the atomic-sphere-approximation the basis is even recalculated for every iteration of the self-consistent cycle. Here only a summary of the concepts will be given and for a more complete description the references\textsuperscript{5,6} are recommended.

The potential at every site in the KKR-ASA method is always taken to be the spherical average of the potential that is obtained by eq. 2.5 inside the muffin-tin sphere. The potential is set to be constant outside the muffin-tin. The basis set may then be constructed as follows:

\[ \chi(\epsilon, r) = \begin{cases} \varphi(\epsilon, r) + P(\epsilon)J(r) & |r| \leq S_M \\ K(r) & |r| > S_M \end{cases} \] (2.7)

where the energy \( \epsilon \) is not calculated but rather included as an input parameter. The resulting radial wavefunctions are then energy dependent. Inside the muffin-tin sphere \( S_M \), the basis function \( \chi \) is a linear combination of the solution \( \varphi \) to the radial Schrödinger equation and solutions to the Helmholtz equation \( J(r) \) outside the muffin-tin sphere. These solutions to the Helmholtz equation are well behaved inside the muffin-tin but diverge when \( |r| \to \infty \). The basis function outside the muffin-tin is then the solutions \( K(r) \) to the Helmholtz equation that diverge when \( |r| \to 0 \). The requirement that \( \chi(\epsilon, r) \) is continuous and differentiable at the muffin-tin sphere boundary and the particular form of \( J(r) \) and \( K(r) \), gives the following formula for the energy dependent coefficients \( P(\epsilon) \):
2.2. The KKR-ASA Green’s function method

\[ D(\epsilon) = \left. \frac{S_M}{\varphi(\epsilon, S_M)} \frac{\delta \varphi(\epsilon, r)}{\delta r} \right|_{r=S_M}, \]  

\[ P(\epsilon) = 2(2l + 1) \frac{D(\epsilon) + l + 1}{D(\epsilon) - l} \]  

(2.8)

where \( l \) is the orbital quantum number.

The total wave function for the crystal is then obtained by a summation over muffin-tin basis functions from the whole lattice as

\[ \tilde{\psi}(\epsilon, r) = \sum_R c(\epsilon) \chi_R(\epsilon, r) \]  

(2.9)

where \( c(\epsilon) \) are the expansion coefficients. The resulting wave function then automatically fulfills the Bloch theorem but does not solve the Kohn-Sham equation unless the added functions \( P(\epsilon)J(r) \) inside \( S_M \) are canceled by incoming tails from \( K(r) \) functions at neighboring sites. This is easy to understand since we know that the solution inside \( S_M \) has to be \( \varphi(\epsilon, r) \). In order to find the solutions to this “tail-cancellation” condition, \( K(r) \) at site \( R \) is expanded in terms of the \( J(r) \) solutions from all other sites as

\[ K_R(r) = -S_{R,R'}J_{R'}(r') \]  

(2.10)

where \( S_{R,R'} \) is the structure constant matrix that contains the information about the lattice. It is independent of lattice parameter as well as energy in the KKR-ASA and LMTO-ASA methods and may therefore be calculated once and for all for every structure. The solution outside the muffin-tin sphere can in general be taken as a linear combination of the \( K(r) \) and \( J(r) \) functions and consequently the structure constant will depend on the coefficients in this linear combination. The linear combination that gives the most localized structure constant is called the tight binding (TB) representation. In this case the functions outside the muffin-tin sphere diverge at large \( r \) and the structure matrix is therefore localized in space. It is normally nonzero only in about 7 atomic shells for the fcc lattice in the TB representation.

Now, the tail cancellation condition has non-trivial solutions for the energies \( \epsilon = \epsilon_i \) where

\[ \det[P_R(\epsilon)1_{R,R'} - S_{R,R'}(k)] = 0. \]  

(2.11)

This is the central equation within the KKR-ASA method and is often referred to as the KKR-ASA equation. However, in practice it does not have to be
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solved in the iteration process in the implementation of the method. Instead
the auxiliary Green’s function is introduced by

\[ [P(\epsilon) - S(k)]g(k, \epsilon) = 1 \Rightarrow g(k, \epsilon) = [P(\epsilon) - S(k)]^{-1} \] (2.12)

and its real space counterpart can be calculated as

\[ g_{R,R'}(\epsilon) = \frac{1}{V_B Z} \int_{BZ} [P(\epsilon) - S(k)]^{-1} \times e^{i\mathbf{k}(R-R')} \, dk. \] (2.13)

This “small” Green’s function is related to the “big” Green’s function \( G(r, r', \epsilon) \)
that solves the actual Schrödinger equation by a transformation that here is just
formally denoted * \( G(r, r', \epsilon) = T[g_{R,R'}(\epsilon)] \) where \( T \) is the transformation op-
operator (for a detailed formula, see eq. 9 in ref. 9).

All physical quantities may now be calculated from \( G(r, r', \epsilon) \), as for example
the charge density. It is obtained from the on site elements of the Green’s
function through the formula

\[ n(r) = -\frac{1}{\pi} \int_{-\infty}^{E_F} \text{Im} \, G(r, r, \epsilon + i\delta) \, d\epsilon \quad \delta << 1 \] (2.14)

and from the charge density, the potential may be obtained as usual from eq.
2.5. The potential is then modified by taking the spherical average and re-
inserted in eq. 2.7. This process is then repeated until self-consistency. The
principal steps in this loop are shown schematically in fig. 2.2.

2.3 The coherent potential approximation (CPA)

The CPA is an approximation to the problem of describing a random substitu-
tional alloy. By random means that the probability of finding one type of atom
at a particular site is determined only by its concentration and substitutional
simply means that there exists an underlying crystal lattice where the atoms
are distributed. A random substitutional alloy may in general consist of many
different kinds of atoms but for simplicity only binary alloys will be discussed
here.

Even with only two types of atoms in the alloy (A & B), all sites in the
system will be different since every position has a unique combination of A
2.3. The coherent potential approximation (CPA)

\[ n(r) = \int_{-\infty}^{E_F} \text{Im} \, G(r, r, \epsilon + i\delta) \, d\epsilon \]

\[ V_{\text{eff}}(n(r)) = V_{\text{act}} + \int \frac{2n(r')}{\gamma(n(r) + \delta_{\infty}(n(r)))} \frac{\delta(n(r') - n(r))}{\delta n(r)} \, d\epsilon \]

\[ D(\epsilon) = \frac{S_M}{\varphi(\epsilon, S_M)} \frac{\delta \varphi(\epsilon, r)}{8\pi} \, \Gamma \left( \frac{l+1}{2} \right) \]

\[ P(\epsilon) = 2(2l + 1) D(\epsilon) \]

\[ g = \frac{1}{V_{\text{box}}} \int_{\text{box}} \frac{|P - S|^{-1}}{e^{i(k - \bar{k}) \cdot \delta \epsilon}} \, d\epsilon \]

**Figure 2.2:** The flowchart for a self-consistent solution of the KKR-ASA equation. Read from top to bottom. If there is no arrow, the next step is into the touching box.

and \( B \) atoms in its surrounding. A simplification of the problem would then be if there was a way to describe an “average” atom that had the properties of the whole system. It is not a straightforward process to perform an “average” calculation and caution must be taken. In fact, it can be shown that there are local properties that can not be averaged in order to describe the whole system. Such properties are said to be non self-averaging. For example the Kohn-Sham single particle wave functions and the atomic potentials are non self-averaging quantities. A DFT method based on a Hamiltonian solution of the Kohn-Sham equation can thus not treat an alloy by considering an average wavefunction or average atomic potential. Fortunately, the total energy, density of states and the on-site Green’s function are self-averaging quantities and this makes the KKR-ASA method very suitable for treating alloys.

An approach to the alloy problem is to replace the random configuration of atoms on the lattice by effective atoms that describe the average properties of the system. These atoms are then said to represent the effective medium of the alloy. The atoms \( A \) and \( B \) are then inserted into the effective medium and treated as impurities. The method to calculate the effective medium in the Green’s function formalism is based on a multiple scattering argument that states the following:

*An electron is propagating in the effective medium. When it arrives at the impurity it will have an additional scattering, but since the effective medium is constructed by the average of the impurities \( A \) and \( B \), this additional scattering must vanish on average.*

The on-site element of the Green’s function is describing the scattering properties of an embedded atom in its surrounding and the above argument then
Chapter 2. The theoretical methods

leads to the equation

\[ 0 = cg_A + (1 - c)g_B - \tilde{g} \Rightarrow \tilde{g} = cg_A + (1 - c)g_B \] (2.15)

where \( c \) is the concentration of \( A \) atoms in the alloy, \( \tilde{g} \) is the auxiliary Green’s function for the effective medium and \( g_{A,B} \) are the auxiliary Green’s functions for the embedded atoms \( A \) or \( B \) in the effective medium. In analogy with the KKR-ASA equation, the Green’s function for the effective medium may be written as

\[ \tilde{g} = \frac{1}{V_B Z} \int_{BZ} \left[ \tilde{P} - S \right]^{-1} \times e^{i(k(R - R'))} d\mathbf{k} \] (2.16)

where \( \tilde{P} \) is the coherent potential function that describes the effective medium. When the effective medium is known, the Green’s functions of the embedded \( A \) and \( B \) atoms are obtained through the Dyson equations

\[ g_{A,B} = \tilde{g} + \tilde{g} \left[ \tilde{P} - P_{A,B} \right] g_{A,B}. \] (2.17)

If equations 2.15 and 2.17 are combined, it is possible to solve for \( \tilde{P} \) and land at the expression

\[ \tilde{P} = cP^A + (1 - c)P^B + [P^A - \tilde{P}]\tilde{g}[P^B - \tilde{P}]. \] (2.18)

Here we can see why the potential function is non self-averaging since the coherent potential is not just a linear average of the two element specific potentials but also contains the extra non-trivial term. However, if the scattering is weak, or equivalently that one of the differences \([P^A - \tilde{P}]\) or \([P^B - \tilde{P}]\) is close to zero, the linear average is valid and more approximate methods should work well.

Equations 2.15 and 2.18 are called the CPA equations and must be solved self-consistently inside the KKR-ASA loop. The idea of the whole KKR-ASA-CPA cycle is shown simplified in figure 2.3. The starting point is in the upper right corner of the figure where the starting guesses for the atomic densities \( n_{A,B} \) are inserted. From these densities the atomic potentials are constructed in the next box by applying eq. 2.5. The next step is to solve the radial Schrödinger equation to obtain the solutions \( \varphi(\epsilon, r) \) inside the muffin tin (not shown). In the next box, the potential functions \( P_{A,B} \) are constructed so that the solutions are continuous and differentiable at the muffin tin sphere boundary.
2.3. The coherent potential approximation (CPA)

\[ n_{A,B}^{A,B}(r) = \int_{-\infty}^{R} \text{Im} G_{A,B}^{A,B}(r, r', \epsilon + i\delta) dr' \]

\[ V_{n_{A,B}^{A,B}}(n_{A,B}^{A,B}(r)) = V_{\text{ext}} + \frac{2n_{A,B}^{A,B}(r')}{|r - r'|} \delta_{r, r'} \]

\[ D(s) = \sum_{\epsilon = s_{M}} \delta \frac{p_{A,B}(s, \epsilon, \epsilon)}{g^{A,B}(\epsilon, \epsilon, r')}, \quad p_{A,B}(s) = 2(2l + 1) \frac{D(s) + l + 1}{D(s) - l} \]

\[ G^{A,B} = \tau[g^{A,B}] \]

\[ g^{A,B} = \bar{g} + \bar{g}[P - p_{A,B}]g^{A,B} \]

\[ \bar{g} = \frac{1}{V_{B}Z} \int_{R_{B}} [P - g]^{-1} \times \frac{1}{\epsilon/k(R - R') dR} \]

\[ \bar{P} = cP^{A} + (1 - c)P^{B} + \frac{[P^{A} - P]g[p_{A} - P]}{|P^{A} - P|g[p_{B} - P]} \]

**Figure 2.3:** The flow chart for a self-consistent solution of the KKR-ASA-CPA equation.

At this stage, the quantities \( P^{A} \), \( P^{B} \) and \( S \) are known and as a starting guess for the gray “CPA-box” in figure 2.3 one can take \( \bar{P} = cP^{A} + (1 - c)P^{B} \) to start the CPA cycle. In the next iterations the choice is of course the old \( \bar{P} \) from the previous iteration. Inside the CPA box, the Green’s function for the effective medium is calculated according to eq. 2.16 and then inserted into 2.18 to re-calculate the coherent potential. The process is repeated until convergence in both \( \bar{g} \) and \( \bar{P} \).

Once self-consistency is obtained in the CPA-box, the embedded Green’s functions are obtained through eq. 2.17 and then transformed into “big” Green’s functions through the same transformation as in the KKR-ASA case. After that, the charge densities for the embedded atoms are calculated by eq. 2.14 and the cycle is completed. Finally, when the charge densities \( n_{A,B} \) do not change from iteration to iteration, the self-consistent solution is found.

In the CPA implementation that was used in this thesis a more general CPA equation than equation 2.18 was used that can handle multicomponent alloys with more than two types of atoms. For a detailed description of this extension, see ref. 10.
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Chapter 3

The magnetic interlayer coupling

3.1 Introduction

The magnetic interlayer coupling was first discovered in 1986 by Grünberg and coworkers as a nonparallel alignment of the magnetization of Fe layers separated by a Cr layer. Later, Parkin and coworkers found that the coupling oscillated as a function of Cr layer thickness. The layer that separates the magnetic layers is usually referred to as a spacer layer, and this will be adopted from now on. Oscillating interlayer coupling has been found to be a general property of magnetic multilayers where the spacer can be almost any metal, ranging from antiferromagnetic spacers to rare-earth spacers and even some non-metallic spacers. A typical setup of a multilayer system and the orientations of the magnetic layers is shown in figure 3.1 a). The strength of the magnetic interlayer coupling for a certain spacer thickness \( N \) is defined as

\[
J(N) = E_{tot}^{AFM}(N) - E_{tot}^{FM}(N)
\]  

where \( E_{tot}^{AFM}(N) \) is the total energy of the system in the case of anti-parallel alignment between the magnetic layers and \( E_{tot}^{FM}(N) \) is the total energy in the case of parallel alignment. The formula 3.1 is defining the bilinear interlayer coupling. In general the magnetization direction of one layer may change continuously with respect to the other layer (see for example reference).

In this thesis, only the bilinear coupling through metallic spacers has been investigated. The model that will be discussed below is a quite simplified version of the quantum well model and it will serve as an introduction to the topic and give perspective to papers I - VI.
3.2 The quantum well model

Quantum confinement

When different materials are put together into a multilayer structure, every propagating state in one of the materials will eventually reach an interface (except the ones that propagate exactly parallel to the interfaces). In order to propagate into the new material on the other side of the interface, there must exist allowed states at that side with the same symmetry. If not, the state is reflected. In general, all states are both reflected and transmitted at the interfaces with some probability that depends on the amount of overlap between corresponding states in the two materials. If one assumes large thicknesses of the layers in the system, it is valid to consider the bulk band structure and estimate the reflection and transmission from the band matching of the materials.

In order to simplify the picture and still capture most of the relevant physics it is sufficient to consider only complete reflection or complete transmission. Consider the simple schematic band structure that is drawn in figure 3.1 b). The bands of the magnetic material are completely spin polarized so that the minority band is unoccupied. If the total magnetization of the layer is ↑, then the majority spin is ↑ as is the case in the left section of figure 3.1 b). In the middle section the band structure of the paramagnetic spacer is shown and then the spin-↑ and spin-↓ bands are degenerate. In the right section is the band structure for the magnetic layer drawn in the case when the total magnetization of that layer is ↓.

First consider the spacer material in the case when the magnetic layers on each side are aligned AFM to each other. Then a spin-↑ electron in the spacer will not have any spin-↑ states to the right to propagate into, since the corresponding band there is located above the Fermi energy. The situation is different on the left hand side where there are possible states to propagate into and the electron may escape into the magnetic material. The same situation will occur for a spin-↓ electron with the difference that it will escape to the right (see figure 3.1 c)). Generally, the scattering at the interfaces will of course change the band structure of the spacer material but in this model we will disregard this fact and consider the band as identical to the bulk band in

![Figure 3.1: A schematic picture of a multilayer structure.](image-url)
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the AFM case. The largest consequence of this approximation is that the surface energy of the introduced interfaces is neglected. This will be evident in the evaluation of the interlayer coupling below.

Now consider the case with ferromagnetically (FM) ordered magnetic layers and consider a spin-$\uparrow$ electron in the spacer. The situation is identical on both sides and it may escape into either side (see figure 3.1 d)). In the model, the band structure for this electron is also assumed to be identical to the bulk band. Since the situation is then exactly the same for spin-$\uparrow$ electrons in the AFM and FM cases, they give no contribution to the energy difference in the equation for the interlayer coupling (equation 3.1). Hence, to model the interlayer coupling, only the spin-$\downarrow$ electrons need to be considered. The spin-$\downarrow$ electrons in the FM case are trapped due to the missing states in the magnetic layers on both sides. The situation is then very similar to the quantum well (QW) problem in quantum mechanics and this is the reason for the name of the model. The trapped electron in the spacer must still follow the bulk band dispersion but the multiple reflections at the interfaces implies an additional boundary condition that will be discussed below.

The continuous case

In the AFM alignment, only the continuous band energy for the spin $\downarrow$ electrons will be considered as discussed above. First some simplifications: The bands will be simplified by considering the electrons in the spacer as freely propagating without feeling any atomic potentials. Then the energy of an electron is $E(k) = \hbar^2 k^2 / 2m$, but to illustrate the interlayer coupling, a special choice of units may be done to obtain the simplified relation $E(k) = k^2$ for the spin $\downarrow$ band. In that case the density of states ($D(E)$) and number of states ($N^p(E)$) in the band becomes (in one dimension)

$$
D(E) = \frac{dE}{dk} = \frac{1}{2\sqrt{E}}
$$

$$
N^p(E) = \int_{-\infty}^{E} D(E) dE = \sqrt{E}.
$$

(3.2)

In particular, the number of states in the entire band for a spacer thickness of $N$ layers is $N \times N^p(E_F) = N \sqrt{E_F} = N k_F$. The total energy of the spacer with $N$ layers becomes

$$
E_{tot}^{AFM}(N) = N \int_0^{E_F} E D(E) dE = N \frac{1}{3} E_F^{3/2} = N \frac{1}{3} k_F^3.
$$

(3.3)
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The quantized case

In the FM alignment, the multiple reflections of the trapped electrons in the spacer implies that only electronic states with wavelengths that are compatible with the width of the well will survive. In figure 3.2 the first four states that survive are drawn. The index \( n \) denotes the states. The wavelengths and the corresponding wave numbers are easily calculated from the figure by counting the number of wavelengths that fit

\[
\lambda_n = \frac{2D}{n} \Rightarrow k_n = \frac{2\pi}{2D} n.
\]  

(3.4)

In for example fcc(001) and bcc(100) multilayers, the well consists of \( N \) atomic layers that are separated by a distance \( \frac{a}{2} \). Then the allowed wave numbers are

\[
k_n = \frac{2\pi}{a} \frac{n}{N},
\]  

(3.5)

In a unit-saving manner we may now assume \( a = 2\pi \) and calculate the sum of the occupied states in the well as the sum

\[
E_{QW}(N) = \sum_{n=1}^{n_{\text{max}}} \left( \frac{n}{N} \right)^2 = \frac{n_{\text{max}}(n_{\text{max}} + 1)(2n_{\text{max}} + 1)}{6N^2}.
\]  

(3.6)

Here \( n_{\text{max}} \) denotes the highest occupied energy level in the well and may be calculated by

\[
E_{n_{\text{max}}} \leq E_F \Rightarrow \frac{n_{\text{max}}}{N} \leq k_F
\]  

(3.7)

Equation 3.6 is decaying with increasing \( N \) as long as no new quantum well level falls below the Fermi energy, that is as long as \( n_{\text{max}} \) is constant. At a certain thickness, \( n_{\text{max}} \) increases with one and there is a discontinuous jump in \( E_{QW}(N) \). This jump in energy is the origin of the oscillatory form of the coupling. The period \( (P) \) is easily calculated as the number of layers that has to be inserted in the well before \( n_{\text{max}} \) is increased. From equation 3.7 in the large \( N \) limit the equals sign holds, and one obtains

\* The special choice of simplifying units for \( k \) in this derivation may be confusing. Another choice is \( k = \pi n/(dN) \) which gives \( P = \pi/(dk_F) \) that is general for any multilayer. The choice of units made here is only done to emphasize the important parameters that influence the interlayer coupling.
3.2. The quantum well model

\[ 1 = (n_{\text{max}} + 1) - n_{\text{max}} = (N + P)k_F - Nk_F = Pk_F \Rightarrow P = \frac{1}{k_F}. \]  

(3.8)

The missing states

It is very important to observe that the energy in equation 3.6 is not the whole contribution to the total energy of the quantum well. The reason is that the number of states in the well is different in the FM and AFM cases. In the AFM case the number of states is \( Nk_F \) as derived in equation 3.2, but in the FM case the number of states is \( n_{\text{max}} \). Since \( n_{\text{max}} \) is always smaller than \( Nk_F \) there are \( Nk_F - n_{\text{max}} \) missing states in the quantum well that must then be located in the magnetic layers. In a more realistic model, the escaped electrons are no problem to describe since there would exist some free states of the same symmetry and spin at the Fermi level in the magnetic layers where they could be placed. Since the spin-\( \downarrow \) band is shifted higher in this model (actually to infinity by assuming infinite walls of the quantum well) the states may be put by hand at the Fermi level of the other spin band. A reasonable scenario would be that the missing states are actually excited into quantum well states above the Fermi level when the magnetization is switched from AFM to FM alignment and then deexcited by some spin-flip mechanism into the spin-\( \uparrow \) band of the magnetic layer.

The total energy of the quantum well is then

\[ E_{\text{tot}}^{QW}(N) = E_{\text{tot}}^{QW}(N) + (Nk_F - n_{\text{max}})k_F^2 \]  

(3.9)

where the second term is the energy of the missing states that are put at the Fermi energy.

The magnetic interlayer coupling

When the energies for the AFM and FM cases are calculated, the definition of the interlayer coupling is transformed into

\[ J(N) = \frac{N}{3}k_F^3 - \frac{n_{\text{max}}(n_{\text{max}} + 1)(2n_{\text{max}} + 1)}{6N^2} - (Nk_F - n_{\text{max}})k_F^2 \]  

(3.10)

and a plot of this function is shown in figure 3.3 together with the energies for the quantum well states.

The coupling shows a damping with increasing \( N \) that behaves as \( 1/N \). This damping is natural since we know that the quantized levels eventually must evolve into a band and recover the energy of the continuous case. There is also a shift to AFM coupling for all spacer thicknesses (\( J(N) \) is negative).
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Figure 3.3: The magnetic interlayer coupling as found by the quantum well model for a single band in the free electron approximation (filled squares in the upper panel). The choice of $k_F$ is 0.18. In the lower panel are the quantum well states plotted together with the corresponding value of $n_{max}$.

The shift is a consequence of the neglected surface energies in the continuous case and may therefore be regarded as an artifact of the model. Clearly it is not present in real systems since the surfaces give the same contribution to the energy in both FM and AFM alignment. It is also clear from the figure that the coupling is oscillatory and that the period is connected to the occupation of new QW states.

The Fermi surface effect

The model this far has treated the 1-dimensional QW problem. In order to include the fact that it is 2-dimensional surfaces that interact in reality, the Fermi surface must be considered. If $N$ is very large the spacer material will retrieve its 3-dimensional Fermi surface which in the case of free electrons is a sphere. The spacer material is still embedded between the magnetic layers so the electrons on the Fermi surface that have a $k$-vector component perpendicular to the interfaces will participate in the multiple scattering in the QW. The perpendicular component may have any magnitude from 0 to $k_F$. In figure 3.4 a cut through the Fermi surface is shown and some of the Fermi surface spanning vectors with perpendicular components are drawn.

The interlayer exchange coupling must then be calculated for every value of the perpendicular component and summed over the Fermi sphere. The result of this summation is that most contributions will cancel. Only those spanning vectors that are stationary with respect to the parallel component will survive. On the sphere in figure 3.4 that is the diameter of the surface.

The interlayer coupling when the parallel $k$-vectors are taken into account is shown in figure 3.5. The cancellations due to the $k_\parallel$ summation introduces an additional $1/N$ damping on the coupling so that the total damping in the
3.2. The quantum well model

Figure 3.4: The Fermi surface for a free electron gas. A few spanning vectors of different length are shown in the $k_\perp$ direction. A spanning vector may be of maximum length $2k_F$.

Figure 3.5: The magnetic interlayer coupling after integrating over the parallel components of the Fermi surface spanning vectors. The $k$-vector is 0.18. Note the changed damping from figure 3.3. The period that is derived for large $N$ is marked by the arrow. In the solid line $N$ has been taken as a continuous variable.

The case of a spherical Fermi surface is $1/N^2$.\(^{32}\)

In summary the period of the magnetic interlayer coupling is shown to depend on the Fermi surface spanning vector of the spacer material. The damping is shown to originate in both the fact that the energy of the quantum well will converge to the continuous band energy for large $N$ and that a narrowing of the constructive interference area on the Fermi surface will occur with increasing $N$.

In paper II the Fermi surface effect on the magnetic interlayer coupling is studied in detail for a Fe/Cu$_x$Pd$_{1-x}$/Fe system in terms of damping, amplitude and phase. The conclusions for that system is that the effect on the amplitude is observable but the effects on damping and phase are very weak.

In paper I is an exotic mechanism that affects the coupling studied, the exchange enhancement in Pd. This system is very interesting since Pd is on the verge of becoming magnetic and the reason for that is explained by the large DOS at the Fermi level. The large DOS results in a high magnetic susceptibility. When a magnetic perturbation is introduced in Pd there will be a large induced magnetic “tail” in the system that may extend over many atomic shells. For example if an Fe atom is inserted in a Pd crystal the Fe atom itself will have a moment that is about $3\mu_B$ but the total induced moment in the volume that was nonmagnetic without the perturbation will be $12\mu_B$.\(^{33}\) In the case of the investigated multilayer, the exact positions of the induced quantum well states were seen to rule the magnetic response of the Pd spacer and as a consequence, the whole magnetic interlayer coupling. The main conclusions were that the
strong magnetic response was responsible for a FM offset of the coupling as well as a phase shift and an increase of the amplitude.

In paper VII the transport properties through an Fe/Pd/Fe multilayer was investigated. The magnetic states in the quantum well region were seen to give a very strong spin-polarization of the current.
Chapter 4

Surface structure

4.1 Beard vs. multilayer growth

To get a feeling of how thin a multilayer is, and how delicate the experimental situation is to produce these systems, one can make use of a not very well known quantity, the beard-second.\textsuperscript{34} If we assume that a beard grows 7 mm/week it grows 1 mm per day. In one day there are 86400 seconds (60*60*24) so in one second the beard grows about $1.2 \times 10^{-8}$ m (1/86400). In units that are more common in multilayer physics this is 120 Å/s. A standard sputtering setup in the laboratory for growing Fe/V multilayers will grow multilayer films at a speed of about 0.5 Å/s.\textsuperscript{35} A sample is usually about 400 Å thick and takes about 15 minutes to produce, the beard grows the same distance in about 3s!! If multilayer growth is like walking, a beard is like a jet plane that is flying by.

4.2 Multilayer growth

Since the multilayers are of a very delicate nature and of such a small size, the construction is difficult to control. The most important parameter in the manufacturing process is the temperature of the sample substrate (growth temperature). The substrate is the foundation on which the atomic layers are deposited and is usually a material with a very well characterized surface, normally MgO (paper VIII) or a single crystal (papers IX, X and XI). A multilayer that consists of layers of two or more elements on a common lattice is called a superlattice. Typically, superlattices are grown by molecular beam epitaxy or sputtering and the layer-by-layer growth is controlled by RHEED \textsuperscript{*} or Auger spectroscopy. The growth temperature has to be sufficiently high to ensure

\textsuperscript{*}Reflection High Energy Electron Diffraction
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Figure 4.1: The different type of structures that are being considered. a) The ideal, atomically sharp interface is the case when both probability parameters are zero and is symbolized by a deltafunction, b) thickness variation (roughness) and c) interface mixing (alloying). The upper graphs show schematically the positions of the atoms of the multilayer (dark and light atoms). Below each graph in b) and c) we show the probability density of interface defects, and the definition of the parameters, $\Gamma_C$ and $\Gamma_T$, that define their geometrical extent. For a more detailed discussion about the parameters, see section 4.5.

large surface mobility and thereby enabling a layer-by-layer growth, often referred to as Frank Van der Merwe growth. At the same time, the temperature must be sufficiently low to prevent the metals from interdiffusing completely and thereby forming random alloys. This delicate balance between surface and bulk mobility is investigated in paper VIII and is of uttermost importance since, as we shall see, all properties that are special for multilayers (interlayer exchange coupling, magnetic moment and critical temperature) depend on the interface quality.

An ideal layer-by-layer growth is then never obtained and all samples suffer from defects such as vacancies, interface roughness and interface intermixing (paper III) as well as misfit dislocations. The energetics and anisotropies of steps on surfaces were discussed in paper XII and XVII. For most material combinations, there is only a small temperature window where the balance between surface and bulk mobility is optimal for superlattice growth. In magnetic superlattices, thickness variation from the interface roughness and interface mixing are the most common types of imperfections. These types are schematically illustrated in Fig. 4.1 and are the type of interface structures that will be discussed in section 4.5.
4.3 Measuring the interface quality

The determination of the atomic structure of materials is a big field in computational materials science and there are many methods that are well adapted to this task. In this context it is important to point out the difference in relaxing a given structure and determining the overall structural ground state of a material. The first case is a problem of finding the equilibrium atomic positions by moving the atoms small distances according to the forces and when the forces vanish the structure is relaxed. The second case involves finding the lattice type that gives the minimum total energy of the system and can mean large displacements of atoms. In a compound it is more complicated and even involves interchanging atoms. The structural ground state is the configuration for which the solution to the Schrödinger equation has a minimal total energy. Both structural effects are detectable experimentally for ordered systems by, e.g., x-ray spectroscopy.

A multilayer is an artificial structure and the positions of each type of atom are partially disordered on the underlying lattice. The concentration wave that describes the multilayer nature of the system only changes in “sharpness” when the interface quality is changed. Since the structure is in between order and complete disorder there is an infinite number of ways to arrange the relative positions of the atoms on the underlying lattice and any attempt to calculate the atomic positions in an energy minimization fashion will fail. If this was done, only the overall structural ground state of the compound would be found. The exact form of the multilayer interfaces depends on how the atoms were “frozen” into the structure.

The exact information about the interface quality is then much harder to obtain experimentally, but there are several ways to obtain qualitative information. The interface structure can be modeled by fitting solutions to Maxwell’s equations to x-ray reflection measurements, scanning-tunneling microscopy (STM) can “see” individual atoms on a surface but cannot see the interface structure inside the material and transmission-electron microscopy (TEM) images are difficult to interpret on a quantitative basis since atomic rows are seen and the concentration is characterized as an intensity. It is also difficult to distinguish between roughness and interface mixing in these techniques. The only experimental tool that can obtain quantitative information about multilayer interfaces to my knowledge is the 3-dimensional atomic probe microscope. Unfortunately there seems to be only a limited number of experiments on multilayer interfaces but the few I have found show beautifully the positions of individual atoms and give very detailed concentration profiles.

In multilayer physics the experiments are of very good quality regarding in- and out of plane lattice constants and average multilayer thicknesses where the uncertainty is usually below 1/100 Å (see paper VIII). From a personal point
of view I find it a remarkable experiment to measure that distance!

4.4 Affected properties

In this section some of the properties that are affected by the interface quality in multilayers will be discussed briefly. In principal all properties of a multilayer that come from the electrons inside the material are changed when the interface quality is changed, but only the particular properties that are investigated in the included papers in this thesis will be treated here.

- **Total energy:** When atoms of two different elements $A$ and $B$ are put together into a multilayer they are “frozen” into that configuration. The resulting artificial structure is then metastable. Depending on the exact growth conditions such as vacuum pressure, substrate quality and deposition rate the “frozen” configuration may differ. Every configuration will have a different solution of the Schrödinger equation and thus a different minimal total energy. The total energy is therefore not sufficient to study in order to determine the interface structure of a multilayer. An example of that is table III in paper IX where a list of total energies for different possible structures of Mn deposited on a Pd fcc(001) surface is given. The energies show that the monolayer of Mn would sink down into the Pd crystal with some structure if the conditions were right. The sample that was studied was first covered with a Mn monolayer at low temperature and then heated for 3 minutes at 570K. The study showed by comparing the calculated DOS with the XES spectrum that one of the structures with intermediate energy in table III was obtained by the heat treatment.

- **Density of states:** The site-projected density of states (DOS) may be compared to x-ray emission and x-ray absorption measurements if the excitation effects are small. That is if the core hole that is created in the experiment does not affect the DOS too much. A core hole is the empty state that is created when a core electron is excited by the x-ray in the experiment. These effects may also be calculated by for example a supercell approach or the $z+1$ approximation. The transition probabilities from core states to band states (the matrix elements) may not vary too much with energy if the DOS should be used to analyze experiments. The probabilities may be obtained by fully relativistic calculations and the transition probabilities were calculated for Fe/Cu by Ebert for the $p \rightarrow s$ and $p \rightarrow d$ transitions. In that study, the $p \rightarrow s$ transition was showed to give only about 5% contribution to the total intensity in the spectrum. For that reason the XAS and XES spectra are normally compared to the partial d-DOS. This was done in papers X, XI and IX for a buried Cu monolayer in Ni, thin layers of Cu on a Ni (100) surface and Mn on a Pd (100) surface respectively. The Cu/Ni results
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Following from the discussion above there is no way to calculate the interface structure of a multilayer theoretically by a minimization of the total energy with respect to the atomic positions (at T=0). In figure 4.2 a multilayer is shown, where the two elements A and B form a random alloy as a ground

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clearly show that the hybridization is strong in the unoccupied part of the DOS for the Cu/Ni interface where the Cu and Ni DOS are indistinguishable from each other but still different from both bulk Ni and bulk Cu. In the Pd/Mn case, the combination of XAS and DOS could even distinguish between different magnetic configurations.

- Core level shift: The pioneering work on the theoretical treatment on the core level shift\(^{46}\) made it possible to include the core hole excitation effects in a natural way in the calculations of the core level shift in alloys and multilayers.\(^{47,48}\) The technique is called the complete screening method and it was used on the Mn/Pd system in paper XIII in order to confirm the results in paper IX and predict the core level shifts for more energetically favorable structures that may be reached in future experiments. It is clear that the core level shift is a very powerful tool where theory and experiment are directly comparable.

- Critical temperature: Critical temperatures have recently been shown to be possible to calculate from first principles theory, by mapping total energy calculations\(^{49,50}\) to a Heisenberg Hamiltonian or by direct calculation using the local force theorem.\(^{51}\) The statistical part of the problem is then solved by means of Monte Carlo (MC) simulations.\(^{50}\) The critical temperature is very sensitive to the surface structure and it was calculated for perfect and rough interfaces in a Fe/V multilayer in paper III.

- Magnetic moments: Hybridization affects the moments strongly in Fe/V multilayers\(^{52}\) and this is the background to the investigations in papers XIV, III,IV and VIII. In bulk the general effects are described by the Slater-Pauling curve, but Niklasson showed that the effect is also detectable at interfaces.\(^{53}\) The general idea is that the intermixing at the interfaces changes the local magnetic moments due to hybridization and the effect may be detectable in the total magnetization of the sample.

- Magnetic interlayer coupling: Since the MIC is an interaction between layers that is mediated by reflections of electrons in a middle layer, the interface roughness is a very important parameter for these systems in general.\(^{38}\) For systems like Fe/V where also the spin polarizations at the interfaces are affected by the interface mixing, the MIC is extra sensitive to the interface structures. The effect on the MIC from roughness and intermixing of the interfaces was studied in papers IV and III.
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state when mixed under the right conditions.

If a multilayer with these two elements was produced in an experiment with the intention to obtain the structure in panel i), the result would probably be similar to one of the middle structures ii) or iii). That multilayer structure would exist just because there are potential barriers to overcome for the atoms in order to change position and reach the ground state configuration iv).

The method that has been explored in this thesis is to use the sensitivities of the properties that were listed in the previous section to find the interface structures of the materials that were investigated. The idea is to find parameters that, when varied, will describe a whole range of possible surface structures and then calculate the property for every structure. In papers VIII, IV, III and XV this property was the magnetic moment of the sample.

As a result there will be one (not necessarily unique) result for every value of the structure parameters. Clearly, at this stage the list of results gives no information about the interface qualities. It is not until the list is compared to one or several experiments that any conclusions about the structure can be made. If the results of many different experiments fit to the same or nearly the same set of values of the interface parameters, then this set is a good candidate to describe the surface structure of the experimental samples. The obtained interface structure may then be checked by using it as input in calculations of other properties. If the new results agree with measured data it is clear that a good enough structure that models the “true” structure has been found.

The interface mixing parameter

In figure 4.1 c) a schematic picture of a multilayer with some degree of interface mixing is shown. The probability density function \( \lambda(X, \Gamma_C) \) (where \( X \) is the position of the interface and \( \Gamma_C \) is a smearing parameter) below the atoms is centered at the position where the ideal interface would be.

If only one interface is considered with many dark atoms to the left and an equal amount of light atoms to the right, the concentration of light atoms
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in layer $N = 1$ that is centered at $X = 0.5$ is obtained by integrating the probability density function from $-\infty$ to $X$ as

$$\Lambda(X, \Gamma_C) = \int_{-\infty}^{X} \lambda(x, \Gamma_C) \, dx.$$  \hspace{1cm} (4.1)

The result is a concentration profile around the interface that may be varied continuously between a step-function ($\Gamma_C = 0$) and a constant line at concentration 0.5 ($\Gamma_C = \infty$). The step-function represents the ideal interface case and the constant line represents the case of complete intermixing.

The particular form of $\lambda(X, \Gamma_C)$ is not known but it can be argued that it should be a Gaussian distribution from the statement of the central limit theorem. The "fuzzy" version of the Central Limit Theorem says:

**The Central Limit Theorem:**

*Data which are influenced by many small and unrelated random effects are approximately distributed as a Gaussian.*

For the rigid version of the theorem and the proof, see reference.\textsuperscript{54} In a more handwaving way it may be argued that the actual form of $\lambda(X, \Gamma_C)$ is not very important since the primary goal is to find a function that describes the evolution from ideal interfaces to the completely mixed case by changing one parameter only.

When the concentration profile for one interface has been calculated the total concentration profile for the multilayer is obtained by summing concentration profiles from all interfaces in the system by

$$C(X, \Gamma_C) = \sum_{i \neq 0} -1^{(|i|+1)} \Lambda_i(sgn(i)X, \Gamma_C)$$ \hspace{1cm} (4.2)

where $\Lambda_i$ is centered at interface $i$. A plot of this function is shown in figure 4.3 together with the most important terms in the summation. At two of the interfaces are the distribution functions $\lambda(X, \Gamma_C)$ shown. As should be clear from this figure, there is nothing that excludes the possibility to assume different distribution functions for the interfaces $A$ on $B$ and $B$ on $A$ in this model.

**The interface roughness parameter**

To construct an easy way to treat the interface roughness, an imaginative experiment will be briefly discussed. Imagine filling a big bathtub with soap-bubbles. The first bubbles that land at the bottom of the tub will spread out when more bubbles arrive from above and at some particular moment in time
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Figure 4.3: The concentration profile of an $A_{3}/B_{13}$ multilayer for $\Gamma_C = 2.0$. Note that $X = N - 1/2$ where $X$ denotes interfaces between atoms and $N$ denotes layer positions.

The bubbles form an almost complete bubble layer. Almost complete is meant that there is a probability that some areas are not yet filled with bubbles and in some places there may be two layers of bubbles. When more bubbles are arriving from above, the holes in the first layer will eventually be filled, but then there is an increasing probability that there will be areas with three or more layers of bubbles. If someone takes a picture of the process of filling the bathtub with bubbles it may look something like figure 4.4.

The point with the above discussion is to give a simplified picture of the growth of a multilayer. To simplify the (mathematical) situation even more, an equal area of holes and islands may be assumed for the surface at every moment in time. If the flow of bubbles is switched off and a new flow of dark bubbles is switched on, the new bubbles will have to grow on the already rough bubble surface. If the flow of dark bubbles is turned off after a while and the old bubbles turned on again, the resulting bubble-multilayer will be very similar to figure 4.1 b). When the flow of bubbles is stopped, the number of bubbles that have fallen into the tub is known with some certainty if the speed of the flow is known and the flow-time is measured. In the real case there would be some atoms that did not land on the desired multilayer surface but on the inside of the vacuum chamber wall and this would produce some uncertainty in the number of deposited atoms. In the bubble case maybe some bubbles plopped and gave the same effect. This means that even if the growth is perfect, the uncertainty in number of atoms will make the last layer incomplete and thereby contribute
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Figure 4.4: A bathtub filled with high quality bubbles that do not break very easily. At this particular moment in time 3 monolayers are completed but totally $\sim 4.2$ monolayers have been deposited.

to the roughness. This effect will be neglected in the roughness model below.

In order to put the probabilities of surface positions into mathematical form a Gaussian probability density function is centered at the position where the ideal interface between dark and light atoms would be in figure 4.1 b). The probability that the interface is deviating $k$ monolayers from the ideal position is then given by the integral

$$P(k, \Gamma_T) = \int_{k-0.5}^{k+0.5} \lambda(x, \Gamma_T) \, dx \quad (4.3)$$

where $\lambda(x, \Gamma_T)$ is the probability density function and the roughness parameter $\Gamma_T$ is the standard deviation. By varying $\Gamma_T$, the range from perfectly flat interfaces ($\Gamma_T = 0$) to equal probability of all interface positions ($\Gamma_T = \infty$) may be described. Clearly the choice to describe the interface roughness by equation 4.3 is just one way to treat many possible interface structures with one parameter. Another choice could be to argue that on a big area of the surface there is a certain probability $\xi$ to deviate one monolayer from the ideal position either as an island or a hole irregardless of where on the surface you are. The resulting probability function would be

$$P(k, \xi) = \left\{ \begin{array}{ll}
1 - 2\xi + 2\xi^2 - 2\xi^3 + 2\xi^4 - \ldots & k = 0 \\
\xi - 2\xi^2 + 2\xi^3 - 2\xi^4 + \ldots & k = \pm 1 \\
\xi^2 - 2\xi^3 + 2\xi^4 - \ldots & k = \pm 2 \\
\vdots & \vdots
\end{array} \right. \quad (4.4)$$

However, in figure 4.5 the two probability functions are compared for some values of $\Gamma_C$ and $\xi$ where the probabilities for $k = 0$ are the same and it may be seen that there is no big difference between the two.
Chapter 4. Surface structure

Figure 4.5: The two probability functions $P(k, \Gamma_C)$ and $\mathcal{P}(k, \xi)$ in the case when $\Gamma_C \simeq 0.7$ and $\xi \simeq 0.4$.

The probability function describes the probability to deviate from the ideal position for one interface. In a multilayer there are many interfaces and the deviations of the individual interfaces leads to thickness variation of each layer. To make the discussion easy only a multilayer consisting of two interfaces will be discussed here. For a more general discussion see paper IV. In the following, this multilayer will consist of $p$ monolayers of $A$ atoms embedded in $B$ atoms.

If a random in-plane position in one interface is picked, the probability to be in the ideal out-of-plane position is $P(0, \Gamma_C)$. If the same in-plane position is picked in the other interface the probability to have the intended thickness of $p$ monolayers is $P(0, \Gamma_C)^2$. The thickness variation formula for the general case is

$$\Theta(t, \Gamma_T) = \sum_{i=-\infty}^{\infty} P(t + i, \Gamma_T)P(i, \Gamma_T) \quad (4.5)$$

where $\Theta(t, \Gamma_T)$ is the probability to deviate $t$ monolayers from the ideal thickness.

**Calculating the property**

The interface mixing is described at an otherwise ideal surface. That means that there is no interface roughness. In order to combine the two imperfections one more assumption must be made, that the islands and holes that are described by the roughness are large compared to the interatomic distances. By making this assumption, the influence from steps and other edge structures such as corners and kinks may be neglected. Then by taking the combination $\{\Gamma_C, \Gamma_T\}$ the situation with intermixing in the interfaces at different positions
Figure 4.6: The surface of total magnetic moment per A atom in, for example, an $A_4/B_6$ multilayer together with the iso-lines of two different experiments. If the iso-lines are projected into the $\Gamma_C, \Gamma_T$ plane they may be compared to iso-lines from other $A_m/B_n$ multilayers and thus the interface qualities may be compared.

is described. To visualize this situation just make the surfaces between the steps in figure 4.1b) very large and then imagine that every surface looks like figure 4.1c).

The idea is to perform calculations of some property ($\omega$) in systems without roughness but including mixing for all possible layer thicknesses. Then the obtained thickness dependent property, for example the total magnetic moment, may be averaged over all thicknesses with the probability $\Theta(t, \Gamma_T)$. The equation for the averaged property ($\Omega$) is then

$$\Omega^{Tot}(p, \Gamma_C, \Gamma_T) = \sum_{t=-\infty}^{\infty} \omega(p + t, \Gamma_C) \Theta(t, \Gamma_T). \quad (4.6)$$

In figure 4.6 the resulting $\Omega(\Gamma_C, \Gamma_T)$ surface is shown for the case when the property is the total magnetic moment per atom in a multilayer. There are also two iso-lines included that symbolize different experiments. The positions of the iso-lines may then be interpreted as an indication that the two experiments were performed on samples with very different interface structures. For a full analysis of real experimental iso-lines, see paper III.
Chapter 5

Modeling magnetism

In order to calculate the desired property for every value of one or both of the interface structure parameters that were discussed in the previous chapter it is desirable to have a very fast model. The model may then be used to estimate the property and narrow the parameter range that needs to be investigated. In both models that will be discussed below are the magnetic moments calculated. In principle any property that depends on the local surrounding may be used such as the core level shift, local DOS etc. The methods are also not restricted to multilayers but may be applied to non-uniform structures in general. It will be shown though that the models work best for disordered structures that are at most partially ordered. The discussion will be about multilayers consisting of two atomic types, A and B.

Both models are based on the fact that atoms are “nearsighted” in a metal. This means that there should be no difference between an atom in the center of a large cluster and an atom inside an infinitely large crystal. That is if the cluster is made large enough and that the local structure around the atom in the crystal and the cluster are identical. This is a statement that is true in principal but it says nothing about the actual size of the cluster that must be considered to obtain a good description of the center atom.

Some information of relevant cluster sizes may be obtained from modern computer codes that use clusters to calculate the properties of materials. The advantage of such approaches are that the computational effort scales linearly with the number of considered atoms. The cluster size that is necessary to consider in these methods depends on the screening length in the material, the atomic structure, the property that is calculated and the boundary conditions of the cluster. A typical cluster size in LSGF is three shells for fcc (46 atoms) and bcc (27 atoms). In LSMS where the boundary condition of the

\[^{\ast}\text{Locally Self Consistent Green’s Function method}^{9}\]

\[^{\dagger}\text{Locally Self Consistent Multiple Scattering method}^{56}\]
cluster is worse, the cluster size may to be about 7 shells to obtain the same accuracy (89 atoms in bcc). In both these methods the electronic structure is calculated self-consistently inside the cluster.

5.1 The local concentration model

In this model the magnetic moment of an atom is assumed to depend only on the concentration of $A$ atoms in the first shell. For a layered structure this local concentration calculated easily as the average concentration of the layers that contain atoms of the first shell. This idea was proposed by Niklasson in the analysis of interface magnetism for ideal surfaces. For fcc (100) the local concentration is

$$C^l_N = \frac{4C_{N-1} + 4C_N + 4C_{N+1}}{12} = \frac{C_{N-1} + C_N + C_{N+1}}{3}$$  \hspace{2cm} (5.1)$$

and for bcc (100)

$$C^l_N = \frac{4C_{N-1} + 4C_{N+1}}{8} = \frac{C_{N-1} + C_{N+1}}{2}$$  \hspace{2cm} (5.2)$$

where $C^l_N$ is the local concentration in layer $N$ and $C_N$ is the layer concentration in that layer. This means that the local concentration and the layer concentration may be different. This is particularly true at a sharp interface. Consider as an example an interface atom at an ideal bcc (100) interface. In this case the layer concentration is 1 but the local concentration is 0.5.

The magnetic moment of a layer is then calculated as

$$M_N = C_N \times m^A(C^l_N) + (1 - C_N) \times m^B(C^l_N)$$  \hspace{2cm} (5.3)$$

where $m^A(B)(C^l_N)$ is the magnetic moment of a bulk $A(B)$ atom in the $A_{C^l_N}B_{1-C^l_N}$ alloy. A plot of $m^A(B)(C^l)$ is shown in figure 5.1. Note that in bulk, $C^l$ is the same as the global concentration $C$. The total moment of a multilayer normalized to the number of magnetic atoms is then the sum over the layers

$$M_{Tot} = \frac{1}{p} \sum_{N} M_N$$  \hspace{2cm} (5.4)$$

where $p$ is the thickness of the magnetic layer.

In figure 5.2 the result of the local concentration model is shown together with self-consistent KKR-ASA-CPA calculations for different amount of interface intermixing in the Fe$_3$V$_{10}$ multilayer. The parameter $\Gamma_C$ is defined in
5.2. The shell environment registry (SER) model

This model is an extension of the local concentration model in order to go beyond the nearest neighbour approximation to describe the local environment. The assumption of the local concentration model is then extended to be that the local property, in this case the magnetic moment, depends only on the local environment up to some shell. In order to take the contribution to the moment from each shell into account properly, it is desirable to have a registry \( m^{A,B}(n_1, n_2, n_3, \ldots, n_i, \ldots) \) that lists the magnetic moments as function of...
local configuration $n_1 \ldots n_i \ldots$ for both atom types. It is of course a bold statement to claim that such a list would be a unique function of the environment since a certain spread that origins in non-local effects is expected. In paper XVI an analysis of the $m^{A,B}$ registry was performed in the case of FeV and indeed a large spread of magnetic moments for similar or even equal shell environments was found. However, the spread that was found in that study should reflect a natural diversity and if the environment registry is handled statistically correct, the average result may still have a meaning. Especially if the structures of the supercells used to obtain the registry are not too far from the structure of the studied system. To obtain a good enough registry of magnetic moments in this study, a large number of small supercells with different concentrations were calculated. The same registry could in principle also be obtained by a few big supercell calculations or one single, carefully chosen, supercell. In the following it is assumed that this list is already calculated. The argument of the registry i.e. the number of atoms in each shell will be denoted as a vector $\bar{n} = (n_1, n_2 \ldots n_i \ldots)$. The registry of magnetic moments is then denoted $m^{A,B}(\bar{n})$.

In the model below only the $A$ atom will be considered. All arguments and formulas naturally also hold for the $B$ atom. The average magnetic moment of the $A$ type of atom at one site in the structure is

$$M^A = \sum_{\bar{n}} P^A(\bar{n}) m^A(\bar{n})$$  \hspace{1cm} (5.5)

where $P^A(\bar{n})$ is the probability that the environment $\bar{n}$ occurs for the considered site. For a given structure, $P^A(\bar{n})$ may be written as a product of probabilities of individual shells

$$P^A(\bar{n}) = \prod_i \varphi^A_i(n_i)$$  \hspace{1cm} (5.6)

where $\varphi^A_i(n_i)$ is the probability to have $n_i$ atoms in the $i$:th shell. The probability $\varphi^A_i$ depends on the actual structure and geometry that is investigated and the forms that are given below are only for $i \leq 2$ in (100) bcc and fcc multilayers with varying concentration profiles of the type that was discussed in chapter 4. In the multilayer it is assumed that there is random disorder within each monolayer. This means that $\varphi^A_i$ is layer dependent and the $n_i$ atoms are distributed over the layers that contain sites within the $i$:th shell. In formulas 5.7 and 5.8 $\varphi^A_1$ is written in the first row and $\varphi^A_2$ in the second row on the right hand side. Every factor on the right hand side corresponds to one layer and the sums are over all possible ways to put $n_i$ atoms in the layers that contain atoms in the $i$:th shell.
5.2. The shell environment registry (SER) model

\begin{align}
\phi^N(n_i) &= \left\{ \begin{array}{l}
\sum_{k \in \mathbb{I}}^4 \left( i \right) C_{N-1}^k (1 - C_{N-1})^{4-k} \times \left( i \right) C_{N+1}^l (1 - C_{N+1})^{4-l} \\
\sum_{k \in \mathbb{I}}^4 \left( k \right) C_{N-2}^k (1 - C_{N-2})^{4-k} \times \left( i \right) C_{N}^l (1 - C_{N})^{4-l} \times \left( i \right) C_{N}^m (1 - C_{N+2})^{4-m}
\end{array} \right. \\
& \vdots \\
& (5.7)
\end{align}

\begin{align}
\phi^N(n_i) &= \left\{ \begin{array}{l}
\sum_{k \in \mathbb{I}}^4 \left( i \right) C_{N-1}^k (1 - C_{N-1})^{4-k} \times \left( i \right) C_{N+1}^l (1 - C_{N+1})^{4-l} \times \left( i \right) C_{N+2}^m (1 - C_{N+2})^{4-m} \\
\sum_{k \in \mathbb{I}}^4 \left( k \right) C_{N-2}^k (1 - C_{N-2})^{4-k} \times \left( i \right) C_{N}^l (1 - C_{N})^{4-l} \times \left( i \right) C_{N}^m (1 - C_{N+2})^{4-m}
\end{array} \right. \\
& \vdots \\
& (5.8)
\end{align}

The probability \( P^A(\bar{n}) \) then also becomes layer dependent and the average magnetic moment of one atom in layer \( N \) is

\[ M_N^A = \sum_{\bar{n}} P_N^A(\bar{n}) m^A(\bar{n}). \]  \hspace{1cm} (5.9)

To obtain the total magnetic moment of an \( A_p/B_q \) multilayer the procedure must be performed for both types of atoms and the obtained element specific total moments averaged with the concentrations in each layer as

\[ M_{Tol} = \frac{1}{p} \sum_{N} C^N M_N^A + (1 - C^N) M_N^B. \]  \hspace{1cm} (5.10)

where the total magnetic moment has also been normalized with the number of \( A \) atoms in the same way as in equation 5.4.

The total magnetic moment per Fe atom in a Fe\(_3\)/V\(_{10}\) multilayer when two shells were included in the \( P \) functions is shown in figure 5.2 together with the local concentration model and self consistent results. The description is improved but the “hump” for sharp concentration profiles is still pronounced. The most possible reason for that is that despite a large shell environment registry most of the environments have zero probability for sharp interfaces. The environments with nonzero probability are rare in the random alloys that were used to obtain the registry and if some important environments are missing, the average magnetic moment will be wrong.
Chapter 5. Modeling magnetism

Figure 5.2: A comparison between self consistent KKR-ASA-CPA calculations, the local concentration model and the SER model of a Fe$_3$/V$_{10}$ multilayer. Both models are a bit off when the multilayer has sharp interfaces but approaches the CPA result for smeared interfaces. In the SER result environments up to second shell were included.

The results in figure 5.2 are a bit surprising considering the results in paper XVI where the individual magnetic moments of Fe atoms in the FeV supercells were investigated and shown to have a large spread even for atoms with equivalent shell environments. Probably, the effects from this spread are partly drowned in the average procedure for smeared interfaces, but may also be responsible for the difference with the CPA results when only very few environments survive.

In summary it can be said that although the simple models that are presented here do not describe the magnetic moments in the Fe/V multilayers to a better extent than within 10-15% in general, they have proved to be a useful tool in estimating the interface mixing parameters to be used in far more accurate and time consuming calculations.
Chapter 6

Conclusions

The problem of determining the interface structure in multilayer physics is very hard. A small uncertainty in interface quality may lead to big variations in the desired properties. Thus it is important to have good control over the manufacturing processes and some easy way to measure the reliability of the resulting multilayer. Especially since the technology moves towards spintronics where the properties of individual electronic states are used. Any disturbances from interface regions in a device may then cause unwanted behaviour.

In this thesis some methods to analyze metallic multilayers have been developed that are based in a close relation between experiments and theory.

It is clear that to solve questions of this kind, it is essential that there is a symbiosis between theory and experiment, not only in terms of information exchange but also in terms of paradigms in the individual scientists that work in this field.
About night orienteering

Orienteering is a sport that is not so well known outside the Nordic countries. It is a single person’s competition where each participant is supposed to find the way to a number of checkpoints in a forest in as short time as possible. As a help you are given a detailed map where the checkpoints are marked. This may not sound too difficult but the fact is that the checkpoint markers in the forest are about 40cm big. They are also put behind some stone or in a shallow hole for example. Often far from roads or footpaths.

A normal age to start competing is when you are about 8-9 years of age.

I am very fond of this sport but it has not always been like that. When I was 8 years old my mother and I went to a beginners course. The theory was easy but it was not the same in practice. The reason is that there are no borders in forests and when I got lost I sometimes went outside the map. Fortunately they had told me to just continue in one direction and then follow the first path or road I found. This tactic sometimes took me in the direction further away from the start but with the help of nice people who took pity on a lost child I always got back in the end. I would like to express my gratitude to them for pointing out directions, offering food and giving me a lift. Unfortunately I do not remember their names.

I also think that my interest in science started in the forest. When you are lost the only alternative is to explore your surroundings in order to figure out how reality is connected to the map. When I finally got a bit more experienced I realized the thrill in actually finding the checkpoints where I expected them to be. The more difficult it seemed to find them when you saw the map, the greater the feeling was to actually find them.

The extreme example of difficulty is the version of orienteering that is con-
ducted in the night-time when, in addition to the map, you are also wearing a headlight. Far from everyone that run orienteering are also running night-orienteering. The reason I like it is possibly because it has a great portion of science built in.

I would like to thank my parents for introducing me to the field of science by encouraging me in my attempts to connect the world to something that is put on paper. You have always supported my fumbling attempts.

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References


A doctoral dissertation from the Faculty of Science and Technology, Uppsala University, is usually a summary of a number of papers. A few copies of the complete dissertation are kept at major Swedish research libraries, while the summary alone is distributed internationally through the series *Comprehensive Summaries of Uppsala Dissertations from the Faculty of Science and Technology*. (Prior to October, 1993, the series was published under the title “Comprehensive Summaries of Uppsala Dissertations from the Faculty of Science”.)