

BACHELOR

Simulating the behaviour of synthetic anti-ferromagnetic NanoPlatelets using COMSOL

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**Simulating the behaviour
of synthetic
anti-ferromagnetic
NanoPlatelets using
COMSOL**

Bachelor Thesis
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Abstract

Nanoparticles show many promising applications, one of which is their use in the field of medicine. In particular, their potential in destroying cancer cells, creating a new tool to deal with this disease. One newly developed kind of particle shows a great promise in this application. Here we investigate this novel particle coined NanoPlatelet which consists of multiple layers stacked upon each other in a configuration of magnetic, non-magnetic and magnetic layers (M-NM-M). This particular stacking results in a perpendicular magnetic anisotropy and anti-ferromagnetic ordering. The goal of this thesis is to create a model using COMSOL multi-physics that simulates the mechanical response of these particles as a function of the direction and magnitude of the magnetic field. Verification of the COMSOL model is done by using a MatLab script, which solves an already existing analytical model.

Contents

Contents	iii
1 Introduction	1
1.1 State of the art	1
1.2 The particles	2
1.3 This thesis	3
2 Theory	5
2.1 Stoner-Wohlfarth model	5
2.1.1 Anisotropy	6
2.1.2 Zeeman interaction	8
2.1.3 Switching field	8
2.1.4 RKKY-interaction	9
2.2 Stoner-Wohlfarth model including RKKY-coupling	9
2.3 Magnetic torque	10
3 MatLab	12
3.1 Double domain Stoner-Wohlfarth model	12
4 COMSOL	16
4.1 Magnetic fields physics	16
4.1.1 Demagnetisation field	16
4.1.2 Torque calculation	18
4.2 Model	20
4.2.1 Geometry	20
4.2.2 Implementation of the Stoner-Wohlfarth model	20
4.2.3 Shape anisotropy	22
4.2.4 Solver	22
4.3 Results	23
5 Conclusions	27
5.1 Outlook	27
Bibliography	29
Appendix	31
A Double domain Stoner-Wohlfarth model	31

Chapter 1

Introduction

1.1 State of the art

The research into nano-sized particles has uncovered many potential applications in different fields. One application for magnetic nanoparticles is treating cancer by mechanical disruption of the cancer cell membrane. Up to now, the most common way of treating cancer using magnetic nanoparticles is using hypothermia, i.e. using heat to destroy the cells. This heat is generated by applying a rapid oscillating external magnetic field to magnetic nanoparticles. This practice has a few drawbacks however, the heat generated is difficult to control. As well as the lack of targeted destruction, since the heat does not distinguish between healthy and cancer cells.

A novel way of dealing with the cells while still destroying them is to utilise a mechanism called apoptosis, which results in suicide of the cancer cell. The way this is achieved is by having nanoparticles exert a torque on the cell-membrane or organelle, which is sufficient to disrupt the cell. This disruption then prompts the cell to destroy itself. The membranes of cancer cells are weaker, and therefore more susceptible to this treatment. Figure 1.1 shows an infographic of the project discussed in this thesis, which starts with the process of cancer cell destruction explained above.

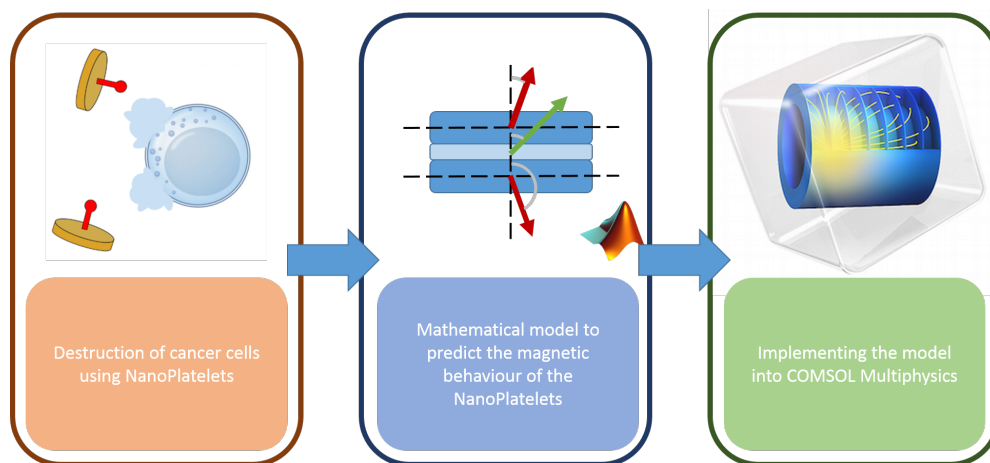


Figure 1.1: Infographic of this project

At the time of writing there are two candidate particles that can achieve this, the first of which is called a vortex particle and the other is called a NanoPlatelet. The name vortex particle is based on the fact that in this nano-sized particle the magnetisation forms a vortex-like structure. The second particle which is a candidate for the method of cancer destruction described above, is the NanoPlatelet. The reason there are only two candidates at this moment, is because not just

any magnetic nano-particle is suitable. For a particle to be suitable, it will need to satisfy two important criteria, which are related to its effectiveness and usefulness in the treatment of cancer.

1.2 The particles

The first criteria is the amount of torque generated by the particle, this needs to be sufficient to disrupt the cancer cell membrane and cause apoptosis. The stronger the torque the more reliable the particle will be in destroying the cell membranes, and thus the cancer cells. However, the torque should be weak enough to not destroy the membranes of healthy cells. The mechanical torque is dependent on the distance from the rotation point, usually the centre of mass, and the force applied to the outer edge. Either the force or this distance can be increased to create a higher torque. This force arises from the interaction of the magnetic anisotropy of the particle and its magnetisation, and thus if this interaction can be changed the force will change as well.

The second criteria is that the particles should not agglomerate in a fluid if there is no magnetic field applied. Therefore the particles need to be able to move towards the region of interest as individual particles. If they were to agglomerate anywhere before arriving at their destination, they would create a solid clump and blocking potential vital areas. To prevent this agglomeration, the particles should not be magnetic in the absence of an external magnetic field. Even better would be particles that are not magnetic when a small field is applied. Most electric appliances, generate stray magnetic fields which could affect how efficient the particles are at travelling to the area of interest in a patient.[8] The next important consideration is the dispersion of the particles once they have fulfilled their goal, for this to happen they should not stay magnetised if the external magnetic field is removed, meaning the particle needs to have a zero remnant magnetisation. The hysteresis loops, showing the magnetic behaviour of the vortex particle and NanoPlatelet, are shown in figure 1.2. The vertical axis shows the magnetisation normalised with respect to the saturation magnetisation, and the horizontal axis shows the strength of the applied field. The red line is the magnetisation when applying a magnetic field in plane of the particle, and the black line is the magnetisation when applying the magnetic field along the axis perpendicular to the plane.

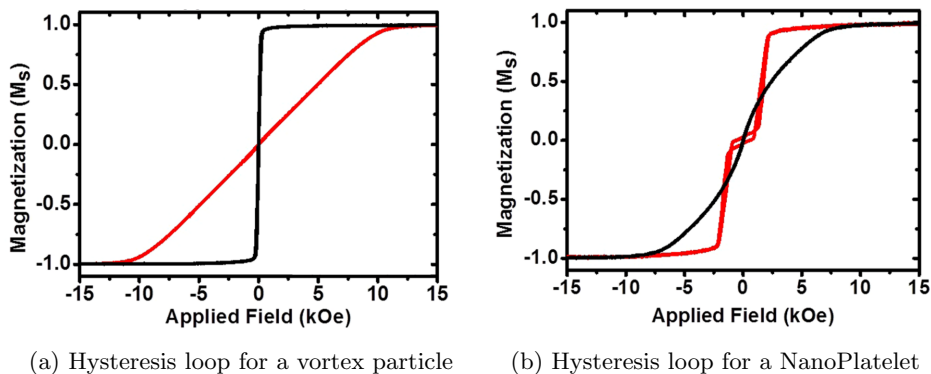


Figure 1.2: Hysteresis loop of the particles, in-plane (black) and out-plane (red). Adapted from Mansell[4]

In figure 1.2a it is shown that for the vortex particle, when applying a magnetic field perpendicular to the particle (red line), the magnetisation results in a gradual slope. Additionally, when applying a magnetic field in-plane (black line) the magnetisation is indeed zero when there is no applied magnetic field. However, just a small increase in the magnetic field strength results in a total magnetisation parallel to the magnetic field. Figure 1.2b shows the the hysteresis loop for the NanoPlatelet, here the in-plane magnetisation shows the sloping behaviour similar to the out-of-plane behaviour of the vortex particle. The out-of-plane magnetisation of the NanoPlatelet is comparable to the vortex particle. For this particle as well, the magnetisation is zero without

an external magnetic field. However, when applying a small magnetic field instead of a sudden complete magnetisation the particle only gets slightly magnetised. This will allow the particle to satisfy the criteria of no agglomeration.

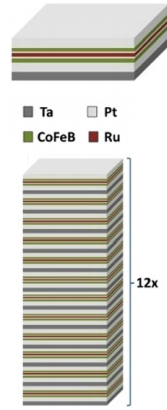


Figure 1.3: Structure of a NanoPlatelet, adapted from Vemulkar [8]. The top structure shows the different layers and the lower one shows them stacked upon each other.

Particles with the specific criteria discussed above are not found naturally, therefore they will need to be fabricated using existing methods, two of which are vapour deposition and sputtering. Since these particles are made artificially, they are called synthetic-anti-ferromagnetic particles. The anti-ferromagnetic part means they have zero total magnetic moment in absence of an external magnetic field. One important difference between the vortex particles and NanoPlatelets is the way they get magnetised (shown in figure 1.4), whereas the vortex has a preference for being magnetised in-plane, the NanoPlatelets actually have a preference to be magnetised perpendicular to its plane. This preference arises from the way the particle is build up, multiple layers that interact with each other, as seen in figure 1.3. This stacking of different materials results in so called perpendicular magnetic anisotropy (PMA) particles.

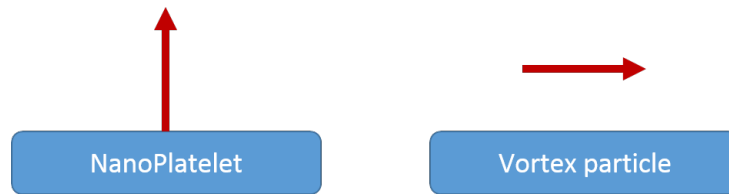


Figure 1.4: Schematic of the preferential direction for the magnetic moment, shown in red. The particle itself is a disc, resulting in axial symmetry.

Research has shows that PMA greatly affects the effectiveness of the particles in the application of destroying cancer cells.[4] Where a tumor treated with vortex particles showed a survival rate of 38% as opposed to 7% for the NanoPlatelets. This is a promising indication for the application of NanoPlatelets in medicine, but there is still a need for more research.

1.3 This thesis

One way to advance this research is to develop a model for the behaviour of these particles and simulate them in the environment of organs or cells. Which is exactly what this thesis is about, to research the possibility of simulating the behaviour of these NanoPlatelets using a COMSOL model in a changing magnetic field. To create a decent model it is needed to understand the physics behind the NanoPlatelets first, which will be discussed in chapter 2 Theory. Because of the complexity of COMSOL, an analytical model will be used first using MatLab before starting to work with COMSOL. This will allow for the results acquired from MatLab to be compared with he results from the COMSOL simulation, as can be seen in the second part of figure 1.1, this analytical model will be discussed in chapter 3 MatLab. After this chapter, the COMSOL model will be created, but first it is necessary to understand how exactly COMSOL works and

what options there are available, this will be discussed in chapter 4 COMSOL. Lastly there is a discussion and comparison of the results, chapter 5 Conclusions.

Because of the complex environment these particles will be active in, the human body, many different physics interact with each other to influence the behaviour of the NanoPlatelets. which is why the model will be created using COMSOL multiphysics, this program allows to couple different physics packages together. This coupling can result in really complex models, combining the fields of magnetism, fluid dynamics and for instance structural mechanics. The aim of this thesis is to create a starting point from which the model can be enhanced, by creating a COMSOL model using an already existing analytical model as a template.

Chapter 2

Theory

This chapter will cover some important physics governing the behaviour of magnetic particles and nanoplatelets in particular. These are the Zeeman-interaction between the magnetic moment ($M[T]$) of the particle and the external applied field ($H[\frac{A}{m}]$), the anisotropy of the particle and the RKKY-interaction between the different layers of the NanoPlatelet. These interactions compete with each other, resulting in a complex energy field. The energy field results in a complex behaviour for the NanoPlatelets as a function of the magnetic field. The RKKY-interaction mentioned before is part of what makes the behaviour of the NanoPlatelets different from the vortex particles, it describes the coupling of two magnetic layers divided by a non-magnetic spacer layer. The mathematical model that will be introduced is the Stoner-Wohlfarth model (section 2.1) and in chapter 4, this model will be implemented in COMSOL multi-physics.

2.1 Stoner-Wohlfarth model

The smallest components of a permanent magnet are the dipole moments of the spin of its electrons, with their own north and south pole. Because of the immense amount of electrons present in the material, which all interact with each other, the computation for each individual magnetic moment would take a long time. To decrease the computation time, it is usually enough to divide the magnet into a few domains that behave as if they were single dipole magnets. The orientation of these domains is what determines if a particle is magnetic or not. The magnetic moment of different domains might cancel each other resulting in a zero net magnetic moment, or they might align themselves with each other which would increase the resulting net magnetic moment.

Because of the size of the particles we are interested in, being on the nano-scale, the magnetic domains are assumed to be approximately the size of the particle. This simplifies some of the physics related to the behaviour of the total magnetic moment. The three important physical phenomena that will need to be taken into account are already mentioned at the start of the chapter: the Zeeman interaction, magnetic anisotropy and the RKKY-interaction.

As mentioned above, the Stoner-Wohlfarth model[1] is used to describe the physics through a numerical model. This will result in a indication of the magnetic behaviour, however there are a few major assumptions that are being made. The first of which is the fact that there are no thermal influences on the magnetic moments, this implies that the model has a temperature of $T = 0[K]$, which of course is not physical feasible as determined by thermodynamics. Another limitation of the model is that it assumes the particle to be fixed and static. This limits the application in a model for the behaviour of a particle, as the NanoPlatelet would not be able to align itself with the magnetic field. This alignment with the magnetic field is interesting, because in further research fluid dynamics might be involved. In which case the orientation can have a big influence on the mechanical behaviour of the particle.

The model uses the energy associated with the different interaction and has as a goal to minimise the total energy, which is done by varying the angle of the magnetic moment with

respect to the particle and external magnetic field. The abstract situation of the SW model for a single magnetic domain particle can be seen in figure 2.1.

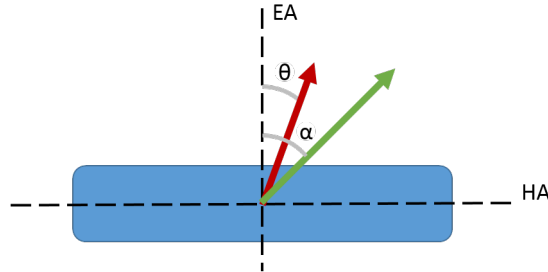


Figure 2.1: Schematic representation of the situation described by the Stoner-Wohlfarth model, showing the orientation of the magnetisation (red) angle θ with respect to the easy axis (EA) and the applied magnetic field (green) as well as its angle α

2.1.1 Anisotropy

Anisotropy is a term used for the dependency of the magnetic moment on direction. A way to think about this anisotropy, is the particle having a energetically favourable state when the magnetic moments of the domain spontaneously align themselves, resulting in a permanent magnet. There are multiple reasons for this preferential alignment, for the Stoner-Wohlfarth model considered here there are two which will be discussed in more detail. The first one is based on the interface of the magnetic material with a secondary material, this will be called the interface anisotropy. The second parameter that influences this direction is the shape of the particle, and is therefore called the shape anisotropy.

This thesis won't be going too much into detail with regards to the interface anisotropy. However, because the NanoPlatelet consist out of thin films, the interface effects are relatively large when compared with the bulk effects. Because of this it is possible to make some assumptions regarding the effects of the anisotropy. The first of which is the direction in which the magnetic moment would align itself if it was the only an-isotropic effect. The situation seen in figure 2.1 is for a particle with a perpendicular magnetic anisotropy (PMA). As discussed in the introduction 1, this is the same anisotropy as with the NanoPlatelets. The direction of the magnetisation in absence of a magnetic field is called the easy axis (EA) and is defined as perpendicular to the work-plane of the NanoPlatelet. Because of this there is a hard axis (HA) in-plane, which is an energetically unfavourable direction for the magnetic moments when no field is applied. Because the NanoPlatelet is shaped like a disk, and the Stoner-Wohlfarth model as described looks at a slice through the middle, it is assumed that the particle is rotational symmetric along the easy axis. This symmetry results in the hard *axis* actually turning into a hard *plane*.

As the name suggests, the shape anisotropy is the directional preference based on the shape of the particle. The reason for the preference is due to the demagnetisation field ($H_{demag}[\frac{A}{m}]$) [7]. This is an internal magnetic field induced by the magnetic moment of the particle. This magnetic field is caused by the electron spins trying to align themselves such that the least amount of magnetic flux lines as possible leave the particle. This effect is the result of magnetic flux lines outside of the material having an energy cost. Take for instance an infinite plane, if the magnetisation is perpendicular to this plane the resulting magnetic flux would all leave the particle, this is less favourable than if the magnetic moment is in-plane. As with the latter situation no magnetic flux lines would leave the (infinite wide) particle. Of course it is not possible to create an infinite plane, but for the thickness on a nano-scale this is an approximation. The field that tries to align the perpendicular magnetic moment with the plane of the particle is called the demagnetisation field. The resulting equation 2.1 takes into consideration the magnetisation as well as a the shape, where the shape is defined as a diagonal 3×3 matrix \aleph . The elements of this matrix represent the

contribution of the magnetisation on the demagnetisation field. The only non-zero elements are on the diagonal, since the x component of the magnetisation has no effect on the demagnetisation field in the y- or z-direction.

$$\vec{H}_{demag} = -\aleph \frac{\vec{M}}{\mu_0} \quad (2.1)$$

Additionally the sum of the diagonal of matrix \aleph is always unity, meaning the demagnetisation field can't be stronger than the magnetisation of the particle. For a sphere, the values on the diagonal are $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}$. This makes sense since the geometry is point symmetric, meaning that there is no preference in either the x-,y- or z-direction. For an infinite wire running along the x-axis the values are $0, \frac{1}{2}, \frac{1}{2}$, this time the symmetry along the wire results in no preference for the y- and z-direction. Lastly for the infinite plane oriented along the x-y work-plane the values are $0, 0, 1$. The magnetic nanoplatelets can be approximated by the infinite plane matrix. The demagnetisation field interacts with the magnetic moment of the particle, equation 2.2 provides a formula for calculating the energy density ($u_s[\frac{J}{m^3}]$) of this interaction .

$$u_{shape} = -\frac{1}{2} \vec{H}_{demag} \cdot \vec{M} \quad (2.2)$$

Here $\vec{H}_{demag}[\frac{A}{m}]$ denotes the demagnetisation field and $\vec{M}[T]$ the magnetic moment vector. However for the NanoPlatelet the demagnetisation field can be described as

$$\vec{H}_d = -\aleph \frac{\vec{M}}{\mu_0} = -\aleph_z \frac{M_z}{\mu_0},$$

since there is only one non-zero ($\aleph_z = 1$) component of the \aleph matrix. Additionally, using the angles defined in figure 2.1 the z-component of the magnetic moment can also be described as $M_z = M_s \cos(\theta)$. Here $M_s = |\vec{M}|[T]$ is the saturation magnetisation of the material. Using these relations and the definition of the dot product, equation 2.2 can be written as:

$$\begin{aligned} u_{shape} &= \frac{M_s^2}{2 \mu_0} \cos(\theta)^2 \\ &= \frac{M_s^2}{2 \mu_0} (1 - \sin(\theta)^2). \end{aligned} \quad (2.3)$$

Because this energy density function will be used to find the minimum energy state, the constant (1) in equation 2.3 will be omitted in further equations. Having worked out the energy density for the shape anisotropy, next is the energy density related to the interface. For this the energy density is defined as:

$$u_{interface} = K \cdot \sin(\theta)^2. \quad (2.4)$$

Here K is the anisotropy constant and θ the angle of the magnetic moment with the easy axis. To get the total energy density related to the anisotropy of the NanoPlatelet, the equations 2.4 and 2.3 are combined into the following equation:

$$\begin{aligned} u_{anisotropy} &= u_{shape} + u_{interface} \\ &= (K - \frac{M_s^2}{2 \mu_0}) \sin(\theta)^2 \\ &= K_{eff} \sin(\theta)^2 \end{aligned} \quad (2.5)$$

For equation 2.5 a new constant is defined, called the effective anisotropy constant:

$$K_{eff} = K - \frac{M_s^2}{2 \mu_0}. \quad (2.6)$$

If $K_{eff} > 0$ the interface anisotropy is greater than the shape anisotropy, resulting in perpendicular magnetic anisotropy. Similarly, if $K_{eff} < 0$ the shape anisotropy is greater than the interface anisotropy resulting in a magnetic anisotropy in-plane of the particle. From equation 2.5 it follows clearly that the anisotropy energy can only be either positive or zero, because of the quadratic sine: $\sin(0)^2 = 0$ and $\sin(\pm\frac{\pi}{2})^2 = 1$. With a maximum anisotropy-energy of K_{eff} when the magnetic moment is perpendicular to the easy axis, and thus parallel with the hard axis (HA).

2.1.2 Zeeman interaction

The physics to be discussed here is the interaction between the magnetic moment ($\vec{M}[T]$) of the domain with the external magnetic field ($\vec{H}[\frac{A}{m}]$). This interaction is called the Zeeman interaction and results in an energy term which greatly increases when these two vectors are not aligned. The result is that the energy can be calculated by taking the dot product of \vec{H} with \vec{M} . Resulting in equation 2.7, where the external magnetic field has a strength $H[\frac{A}{m}]$ and an angle $\alpha[rad]$ with respect to the easy axis.

$$u_{Zeeman} = -HM_s \cdot \cos(\alpha - \theta) \quad (2.7)$$

In this equation the term $M_s[T]$ is the magnetic saturation, $H[\frac{A}{m}]$ the strength of the applied field and $u_{Zeeman}[\frac{J}{m^3}]$ the energy density. It is important to notice the minus sign, this implies that to minimise the Zeeman-energy the term $\cos(\alpha - \theta)$ needs to be maximised. This is the case for $\cos(\alpha - \theta) = \cos(0) = 1$, when magnetic moment and the applied field are aligned parallel. Because of the symmetry of the cosine the Zeeman-energy will be positive when \vec{M} and \vec{H} are anti-parallel ($\alpha - \theta = \pm\pi$), therefore maximising the Zeeman-energy.

2.1.3 Switching field

Combining equation 2.5 and 2.7 we get the equation for the total energy density for one layer:

$$\begin{aligned} u_{total} &= u_{Zeeman} + u_{anisotropy} \\ &= -H M_s \cos(\alpha - \theta) + K_{eff} \sin(\theta)^2. \end{aligned} \quad (2.8)$$

As discussed in section 2.1.1 and section 2.1.2 the position of the magnetic moment \vec{m} is what really impacts the energy of the system. And to minimise this energy the angle of the magnetisation is the variable parameter. From equation 2.8 it is possible to deduce the magnetic field strength associated with the magnetic anisotropy, this field strength is called $H_k[\frac{A}{m}]$. If the external magnetic field is oriented along the hard axis ($\alpha = \frac{\pi}{2}$) this is the field strength needed to align the magnetic moment with the magnetic field.

$$u_{\alpha=90 \text{ deg}} = -H M_s \cos(\frac{\pi}{2} - \theta) + K_{eff} \sin(\theta)^2 \quad (2.9)$$

$$\frac{\partial u_{\alpha=90 \text{ deg}}}{\partial \theta} = -H M_s \cos(\theta) + 2 K_{eff} \sin(\theta) \cos(\theta) = 0 \quad (2.10)$$

$$H M_s \cos(\theta) = 2 K_{eff} \sin(\theta) \cos(\theta) \quad (2.11)$$

$$H = \frac{2 K_{eff}}{M_s} \sin(\theta) \quad (2.12)$$

Starting with 2.9, having set $\alpha = \frac{\pi}{2}$, the partial differential is taken with respect to θ . This is then used to determine the minimum energy equation, by setting equation 2.10 to be equal to zero. This results in the equations 2.11 and 2.12, and lastly the angle θ is of course equal to $\frac{\pi}{2}$ when $H = H_k$. Resulting in the following relation for the anisotropy field $H_k = \frac{2K}{M_s}$.

2.1.4 RKKY-interaction

Section 2.1 has discussed the basic physics implemented in the SW model. However, for the NanoPlatelets this is not enough, they experience an effect called RKKY-interaction[5] named after Ruderman-Kittel-Kasuya-Yosida. This interaction is an example of indirect exchange coupling. For NanoPlatelets this means the magnetic moments of the two magnetic layers are influenced by each other. Because of the nonmagnetic spacer layer between the two magnetic layers the wave functions of the conduction electrons interfere with each other, resulting in scattering and transmission phenomena.

The thickness of the spacer layer is crucial in the behaviour of the RKKY-interaction, since the thickness defines if the layers are either ferromagnetically (F) or anti-ferromagnetically (AF) coupled. Without going too deep into the derivation of the theory, it is interesting to understand how this change in coupling can occur based on the thickness. To do this the RKKY function[6] is needed:

$$F[\xi] = (\sin \xi - \xi \cos \xi) / \xi^4 \quad (2.13)$$

where $\xi[\text{arb.un.}]$ is defined as $\xi = 2k_F r$, with $k_F[\frac{1}{m}]$ the Fermi wavevector and $r[m]$ the thickness of the nonmagnetic layer. One thing to note is the dependency of this equation on ξ^{-4} , such that for larger values of ξ it rapidly approaches zero. Meaning the effect of the RKKY-coupling results in a sizeable interaction compared to the magnetic anisotropy and Zeeman energy for nanometre thin layers.

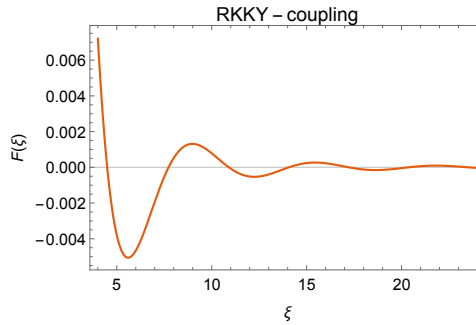


Figure 2.2: Graph showing the result of the RKKY function, the x-axis shows the dimensionless parameter ξ as defined above. The y-axis shows the strength of this function.

Whenever the value of $F[\xi]$ is positive the two layers are coupled ferromagnetically, and if it is negative the coupling is anti-ferromagnetically. The first minimum is at around $\xi = 5.5$ and results in the strongest anti-ferromagnetic coupling.

2.2 Stoner-Wohlfarth model including RKKY-coupling

In this section the Stoner-Wohlfarth including the RKKY-coupling term will be discussed. Figure 2.3 shows an abstract representation of this model, the magnetic layers are shown in dark blue, and the nonmagnetic layer is shown in a lighter blue. The Zeeman interaction and anisotropy of the two magnetic layers are independent, however for this model the parameters $H[\frac{A}{m}]$, $M_s[T]$ and $K[\frac{J}{m^3}]$ are assumed to be equal for the top and bottom layer. Because the parameters are equal they can be grouped together, which would not be possible otherwise. The definition of the different angles can be seen in figure 2.3, with θ_1 being the angle of the magnetisation of the upper layer, θ_2 the angle of magnetisation of the lower layer and α the angle of the applied magnetic field. All these angles are with respect to the easy axis, which is perpendicular to the plane in the case of NanoPlatelets.

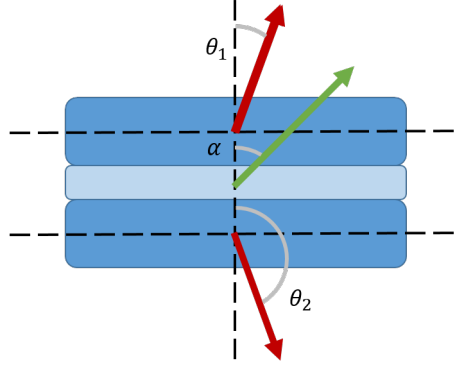


Figure 2.3: Definitions two layer coupled Stoner-Wohlfarth model, magnetic moments are given in red and the applied magnetic field in green.

With the angles defined, the RKKY-coupling can be added. As discussed in section 2.1.4 the energy will be minimal when the magnetisation is anti-parallel, or the difference in angle $\Delta\theta = \pm\pi$. This can be done by taking the dot product of the two magnetisation vectors, or the cosine of the difference in angle, resulting in a positive value when $\Delta\theta = 0$. Taking all the changes for the modified SW model into account results in the following equation:

$$u_{total} = -HM_s \cdot (\cos(\alpha - \theta_1) + \cos(\alpha - \theta_2)) + K_{eff} \cdot (\sin(\theta_1)^2 + \sin(\theta_2)^2) + \frac{J}{t} \cos(\theta_1 - \theta_2). \quad (2.14)$$

Here the first two terms, are the Zeeman energy and Anisotropy energy for the different layers. The third and new term, is the energy associated with the RKKY-interaction. Where $J[\frac{J}{m^2}]$ is a surface energy term, positive in the case of anti-ferromagnetism. This J is proportional to the function given in equation 2.13 but with opposite sign. The energy decreases with the thickness $t[m]$ of the magnetic layer. Therefore the effect of the RKKY-interaction is only at the interface between the magnetic and non-magnetic layer. When increasing the thickness of the magnetic layer, the volume increases and the effect of the RKKY interaction becomes less with respect to the anisotropy and Zeeman energy, since these scale with the volume of the layer. Keeping in mind that the thickness of the non-magnetic spacer layer is fixed, as discussed in section 2.1.4.

As with section 2.1.3 it is interesting to investigate the point at which the magnetic moment is expected to 'switch'. Assuming the magnetic field is along the easy axis, the magnetic moment anti-parallel to this field will need to overcome both the energy associated with the anisotropy as well as the energy associated with the RKKY coupling. This means that the switch field will be a combination of the two, resulting in a new field strength called H_{total} .

2.3 Magnetic torque

In section 4.1.2 a verification will be done for the calculation of the magnetic torque simulated by COMSOL. To be able to compare those results with the theoretical value a short explanation will be provided. First of all the magnetic torque is not the same as the mechanical torque. The latter is the result of a force acting on a point a certain distance away from its rotation axis. The magnetic torque is different in that it acts on the magnetic moment of a material. This magnetic torque is for instance the reason electronic motors can work. The magnetic torque per volume ($\tau[\frac{N}{m^2}]$) is defined as the cross product (\times) between the magnetic moment and a magnetic field:

$$\vec{\tau} = \vec{M} \times \vec{H} \quad (2.15)$$

This equation can be rewritten using the definitions of the Stoner-Wohlfarth model for the magnetic moment and magnetic field resulting in the following equation:

$$\tau[\alpha, \theta] = M_s H (\cos(\theta) \sin(\alpha) - \sin(\theta) \cos(\alpha)) \quad (2.16)$$

Where $\alpha[rad]$ is the angle of the magnetic field and $\theta[rad]$ the angle of the magnetisation. However, to get the total magnetic torque acting on the magnetic moment of a particle, the above equation needs to be integrated over the volume of this particle. Assuming $M_s[T]$ and $H[\frac{A}{m}]$ are not dependent on their position in the particle, equation 2.16 can be multiplied with the volume. The torque is maximum when the difference between α and θ is equal to $\frac{\pi}{2}$. For instance when $\theta = 0[rad]$ and $\alpha = \frac{\pi}{2}[rad]$, equation 2.16 gives the maximum torque to be $T_{max}[N m] = V \tau = V M_s H$.

In this chapter the Stoner-Wohlfarth model for the NanoPlatelets has been discussed, in the following chapter it will be implemented in MatLab

Chapter 3

MatLab

To be able to validate the results obtained from COMSOL simulations a numerical model is used. The Stoner-Wohlfarth model only looks at the particle in two dimensions, while the model created using COMSOL will be three dimensional. This creates an additional degree of freedom for the magnetic moments, which could result in deviations from the two dimensional model. This is something to keep in mind for when comparing the results. This model will be implemented and solved using MatLab. First the model for a single domain is implemented to better understand the effects of the Zeeman interaction and magnetic anisotropy. This is important since the two magnetic layers of the NanoPlatelet each individually behave as a single domain, only by the addition of the RKKY coupling changes it into the full SW model. After the single domain is verified, the double domain coupled by RKKY is implemented. In chapter 4 the double domain Stoner-Wohlfarth model is implemented in a COMSOL model, forming the basis for further modelling.

3.1 Double domain Stoner-Wohlfarth model

This model will describe two magnetic domains coupled using the RKKY interaction, this is done by implementing equation 2.14 and its relevant parameters. The complete MatLab code can be found in appendix A.

The code starts by initialising the relevant parameters, which in the case of the double domain SW model are the saturation magnetisation $M_s = 1[T]$, the effective anisotropy $K_{eff} = 1 * 10^5 [\frac{J}{m^3}]$, the thickness of the cobalt layers $t = 1 * 10^{-9} [m]$ and the surface energy term associated with the RKKY interaction $J = 2.5 * 10^{-4} [\frac{J}{m^2}]$. The saturation magnetisation of $M_s = 1[T]$ implies that the magnetic moment of the top and bottom layer are both $M_{top} = M_{bottom} = 0.5[T]$. Using equation 2.12 it is possible to use the parameters provided to calculate H_k , which results in $H_k = 2 * 10^5 [\frac{A}{m}]$. However this is the switching field if there is no RKKY interaction, and therefore the switching won't happen at a single value for the field strength. There will be four values at which a switch will happen, $H = \pm H_k \pm H_{rkkky}$. The external magnetic field strength will range from $H = -5 * 10^5 [\frac{A}{m}]$ to $H = 5 * 10^5 [\frac{A}{m}]$ in small increments. After each increment the previous equilibrium will encounter a small disturbance to simulate a thermal fluctuation. This is done to give the model a chance to escape a local minimum for a global minimum if the situation occurs. The code will calculate the angle of the upper and lower domain, based on the angle and strength of the external magnetic field. There are a few configurations with which it is possible to predict the expected behaviour of the magnetisation, based on the theory discussed earlier. These different configurations are achieved by varying the angle of the external magnetic field with respect to the easy axis. When there is no external magnetic field ($H = 0 [\frac{A}{m}]$) the magnetic moments of the two layers should cancel each other out resulting in no net magnetic moment.

The first configuration is when the magnetic field is applied perpendicular to the plane, which means it is parallel to the easy axis. For strong magnetic fields ($H = \pm 5 * 10^5 [\frac{A}{m}]$) the magnetic

moments are expected to align themselves parallel to the applied field. To get a better grasp on the situation, the components of the magnetic moment are shown parallel and perpendicular to the easy axis, separated for the upper and lower domain. Figure 3.1 shows the total parallel component for the configuration where the magnetic field is varied along the easy axis. On the y-axis the sum of the magnetic moment is shown, where M_s is the saturation magnetisation for one domain.

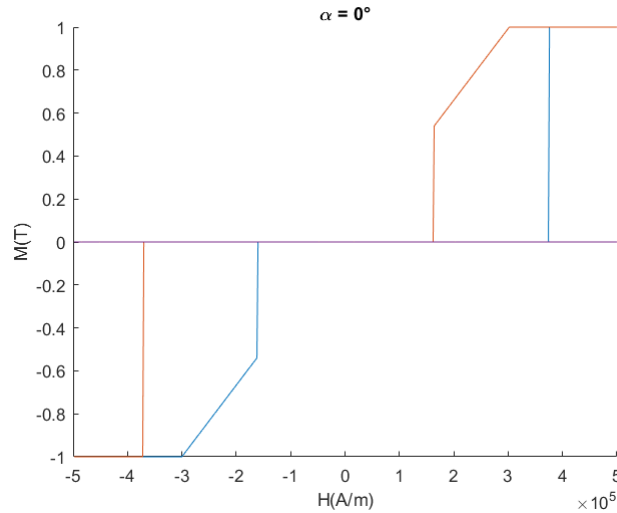


Figure 3.1: This graph shows the total magnetisation for $\alpha = 0^\circ$. The blue line is for increasing the magnetic field, and the red line when the magnetic field is decreased again.

The explanation for the sloping behaviour seen in figure 3.1 is the strong effect of the RKKY coupling compared to the effect of the anisotropy. This means the magnetic moments, being aligned parallel to each other, want to move away from each other more than that they want to be aligned to the easy axis. Which explains the magnetic moment aligning itself partially with the hard axis, as can be seen in figure 3.2 on the top row. This figure shows the projections of the magnetic moment along the hard- and easy axis.

The upper left part of this figure shows the magnetic moment component of the first domain perpendicular to the easy axis, the lower left is the same domain but the component parallel to the easy axis. The blue line shows the effect of increasing the magnetic field from

$$-5 * 10^5 \left[\frac{A}{m} \right] \text{ to } +5 * 10^5 \left[\frac{A}{m} \right],$$

while the red line shows the result for decreasing the magnetic field. It clearly shows that the magnetic moment projected along the hard axis has a non-zero component when the switch happens. Important as well is that for the top and bottom layer they are mirrored, resulting in still a net zero-magnetic moment along the hard axis.

The next configuration used is when the applied magnetic field is perpendicular to the easy axis (or parallel with the hard axis). Again the starting position for $H = 0 \left[\frac{A}{m} \right]$ is with the two magnetic moments cancelling each other. However, by increasing the field strength the Zeeman interaction will start to dominate the energy function. Eventually, when the field is strong enough, the magnetic moments should align themselves along the hard axis. The results for this configuration can be seen in figure 3.3

The magnetic moments along the hard axis agree with the expectations, since they increase linearly with the strength of the magnetic field. The behaviour of the components parallel to the easy axis is actually quite interesting, since it is not as predictable as the previous situation with $a = 0^\circ$. The most noticeable part of the graph is the circular result obtained for the components

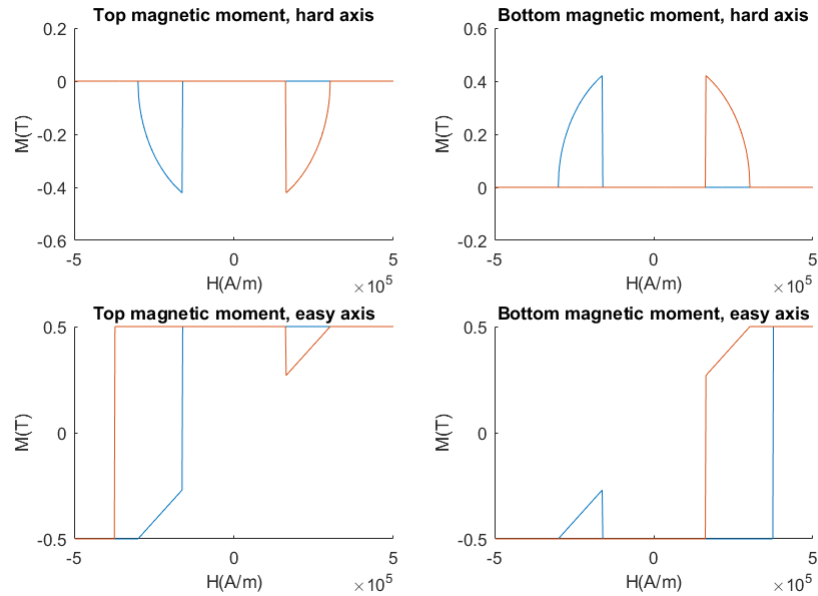


Figure 3.2: This graph shows the different components of the magnetic moments for the top layer (Left) and bottom layer (Right), along the hard axis (Top) and the easy axis (Bottom). The magnetic field is oriented along the easy axis, thus $\alpha = 0^\circ$.

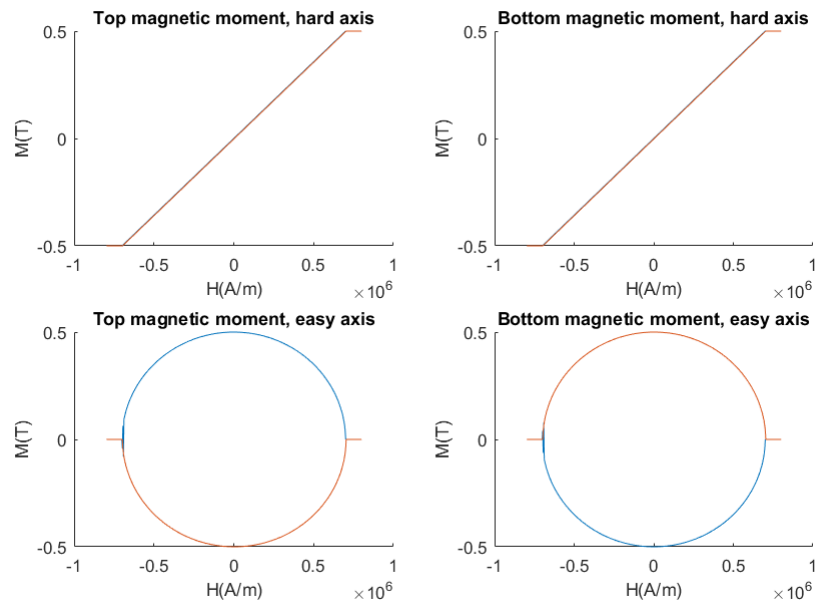


Figure 3.3: This graph shows the different components of the magnetic moments for the top layer (Left) and bottom layer (Right), along the hard axis (Top) and the easy axis (Bottom). The magnetic field is oriented along the hard axis, thus $\alpha = 90^\circ$.

along the easy axis. This makes sense because the anisotropy energy decreases with \sin^2 and the Zeeman energy with \cos , this would explain the circular graph.

Lastly it would be interesting to see what happens when the magnetic field is oriented at an angle of $\alpha = 45^\circ$. For large values of the magnetic field, the magnetic moments are again expected

to align themselves with the field. The simulated magnetic behaviour is shown in figure 3.4.

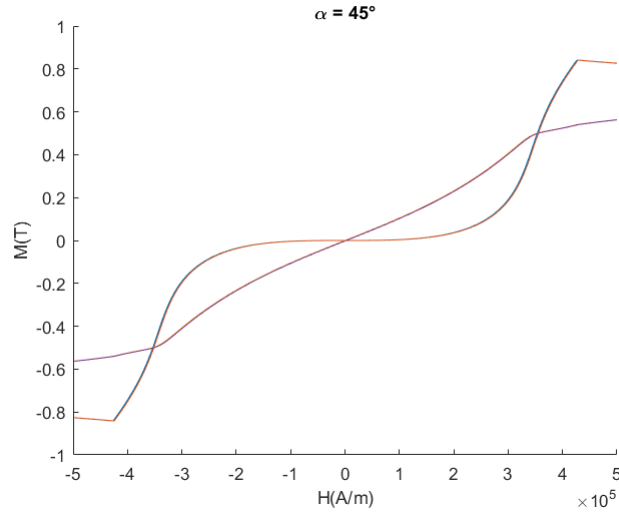


Figure 3.4: Total magnetic moment for an applied field with $\alpha = 45^\circ$. Shown are the components parallel and perpendicular to the easy axis, both for increasing and decreasing fields.

Figure 3.5 shows the magnetic moment along the hard axis increases until it reaches the maximum value of $M_{max} = 0.5[T]$, it then drops off again. This represents the magnetic moment oriented in the opposite direction of the magnetic field switching signs and aligning itself with the magnetic field. For the bottom row the switching is even more clear, as the component along the easy axis switches sign. However unlike with the configuration of $\alpha = 0^\circ$, after the switch the magnetic moment is not aligned completely with the easy axis.

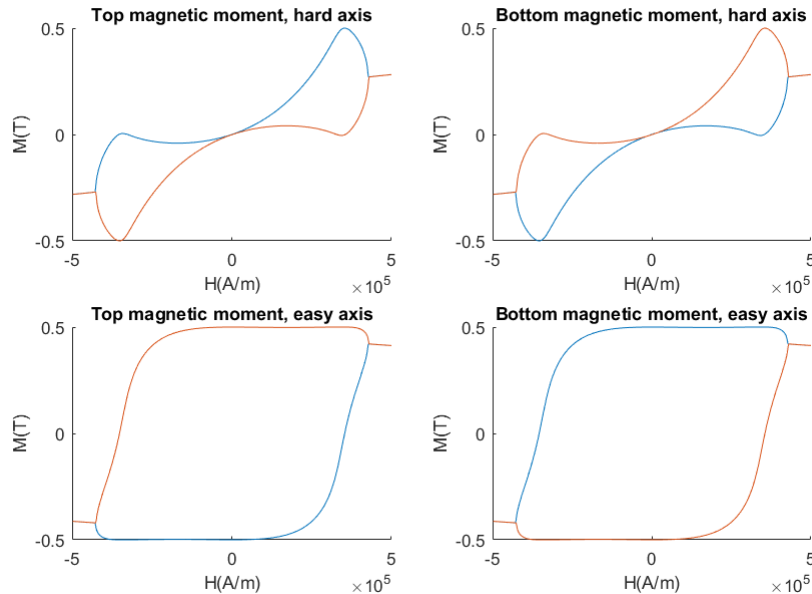


Figure 3.5: his graph shows the different components of the magnetic moments for the top layer (Left) and bottom layer (Right), along the hard axis (Top) and the easy axis (Bottom). $\alpha = 0^\circ$.

Chapter 4

COMSOL

This chapter will cover the program COMSOL, and how it can be used in the modelling of NanoPlatelets. The chapter will start by describing the tools COMSOL provides to model magnetic particles. The magnetic fields package allows for the simulation of a demagnetising field as well as simulating the torques and forces acting on the magnetic particle. Next the created COMSOL model is discussed and the adjustments that had to be made to be able to use the magnetic fields package in the modelling of NanoPlatelets. Lastly the results obtained from simulating the final model for situations similar to the ones discussed in section 3.1 the double domain Stoner-Wohlfarth model using MatLab.

COMSOL is a simulation program that excels in combining different physics in its model. The combination of physics is useful because it allows to first create a model for electromagnetic part of the problem, the interaction between the magnetisation and the magnetic field. And then combine this model with for instance a fluid dynamics package. Assuming both physics are defined correctly, the resulting model is a representation of the behaviour of magnetic nanoplatelets in a cancer cell. This thesis will only describe the reaction of the magnetisation to the external field.

4.1 Magnetic fields physics

The physics package used to model the behaviour of the magnetisation of the nanoplatelets is the magnetic fields (mf) package. The package is used to calculate the magnetic fields and induced current distribution in and around magnets, coils and conductors. The package will be used to approximate the magnetic behaviour of perpendicular magnetised particles. However the package assumes the magnetic particle to be a permanent magnet, which is not sufficient for modelling the magnetic behaviour of the NanoPlatelet.

To add the Zeeman interaction, anisotropy and RKKY interaction, the theoretical SW model is modified in such a way that COMSOL can solve for the desired equilibrium situation. For this, many solutions have been tried, but they were usually only effective in the post processing of the simulated data. The desired solution would be to write a complete new physics package specifically tailored for these interactions. COMSOL does provide the ability to create custom physics packages, but this turned out to be rather complicated and time consuming. COMSOL provides the ability to code your own functions in C, but here the lack of experience in C was a problem. Another potential solution was the optimisation package provided by COMSOL, but this is not included in the base license and it should be possible to solve for without having this package.

4.1.1 Demagnetisation field

As discussed previously in section 4.1.1, the demagnetisation field present in the nanoplatelets is important in the simulation of the magnetisation. To make sure COMSOL is correctly calculating

this field, it will be compared to the theoretical value for three geometries: a plane, a wire and a sphere.

The verification model used is to morph the geometry from a wire-like particle towards a sphere. The model returns the non-zero components on the diagonal of the \aleph matrix. The primitive geometry used for this, is to go from an elongated ellipsoid to a sphere. The simulation will result in a graph showing how the components of the matrix evolve as the geometry changes. The morphing is achieved by using a single parameter ($d_{a,b}$) for the a and b semi-axis of the particle, starting from a small value and increasing this towards the value for the radius of the sphere (R_0), shown in figure 4.1. Taking the $d_{a,b}$ sufficiently small, the resulting geometry is an approximation for the wire situation, seen in figure 4.1a. Arriving at the spherical geometry, the components of the \aleph matrix should be the same as for the theoretical value, as there are no infinite dimensions as was the case for the wire and plate.

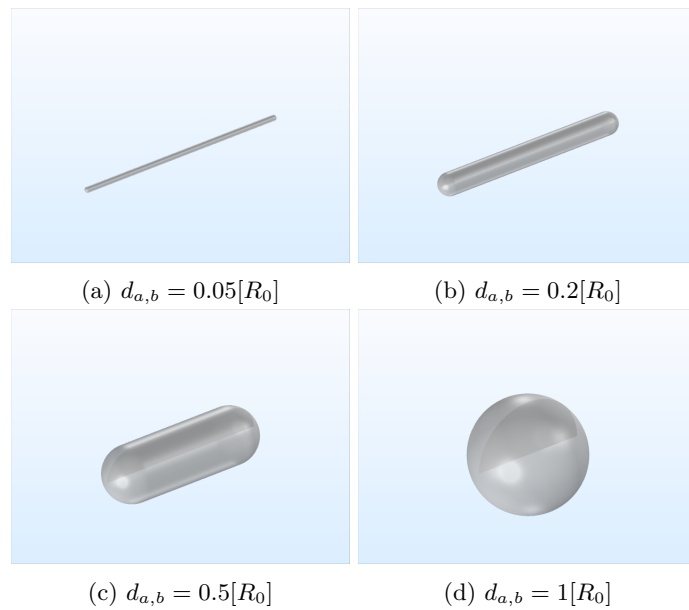


Figure 4.1: Geometry of the particle used in the demagnetisation verification, for different values of $d_{a,b}$

To 'probe' the particle and measure the demagnetisation field, for each iteration of $d_{a,b}$ the magnetic moment of the particle is oriented in such a way that it is first parallel to the x-axis. The demagnetisation field is measured in the model after which the magnetic moment is changed to be parallel to the y-axis, with another measurement. This process is then repeated lastly for the z-axis. Besides magnetisation, there is no other source of magnetic fields, meaning that any fields that do arise will be the result of the demagnetisation field, calculated by COMSOL. To then acquire the components of the tensor, equation 2.1 is written such that $\aleph_i = -\frac{H_i}{M_i}$ for $i = x, y, z$. The results are shown in figure 4.2, where the z- and y-components are so similar that the lines overlap.

As discussed earlier, a snapshot of the geometry for different values of $d_{a,b}$ is given in figure 4.1. Starting with the lowest value for $d_{a,b}$, which is the approximation for the case of a wire. This implies that the demagnetisation field in the x-direction (along the length of the wire) will be zero, and the components in the z- and y-direction are both $\frac{1}{2}$. The results shown in figure 4.2 indeed agree with this prediction. The blue line, which represents the x-component of the matrix, will pass through zero. However, for it to be completely zero the wire would need to be infinite which is not possible for COMSOL. The values for the y- and z-component are close to $\frac{1}{2}$, but not quite since the three values will have to add up to 1. Figure 4.1 shows the different geometries used in the simulation, where 4.1a is the approximation of the infinite length wire and 4.1d is a

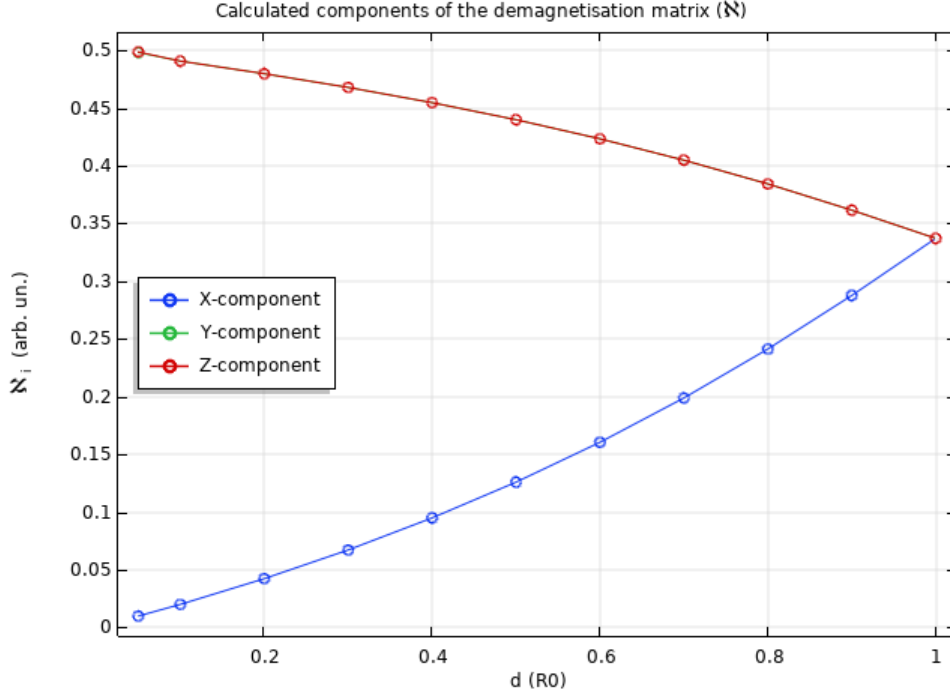


Figure 4.2: Simulated \aleph components for a morphing geometry, the blue line shows the $\aleph_{x,x}$ component of the matrix and the red and green line (which lay on top of each other) show the $\aleph_{y,y}$ and $\aleph_{z,z}$ components.

sphere.

The values calculated by COMSOL for $d_{a,b} = 0.05R_0$ are: $\aleph_x = 0.010$, $\aleph_y = 0.498$ and $\aleph_z = 0.499$. These values are close but not exact to those of a wire $(0, \frac{1}{2}, \frac{1}{2})$, the reason for this is the approximation and the numerical error. The other comparison with theory is for the geometry of a sphere, which theoretically should result in all the tensor components being equal to $\frac{1}{3}$. Figure 4.2 shows that the components clearly do converge to a value approximately $\frac{1}{3}$ for $d_{a,b} = R_0$. Extracting the calculated components from COMSOL, gives: $\aleph_x = 0.337$, $\aleph_y = 0.337$ and $\aleph_z = 0.337$. These components all add up to 1.011, similar to the situation for $d_{a,b} = 0.05[R_0]$. Besides the slight numerical inaccuracy the values are all equal to each other, which should be the case for a sphere $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Meaning there is no directional preference for the magnetisation, as discussed in section 2.1.1.

4.1.2 Torque calculation

One of the most important modules of the magnetic fields package that will be used in the model is the "Magnetic force calculation module", which will calculate the force and torque on a magnetic particle under the influence of an external field. For this equation 2.15 from section 2.3 will be used. From this equation a relation for the maximum torque was deduced, which was

$$T_{max} = V \tau = V M_s H \quad (4.1)$$

The simulation used to verify the calculation of the magnetic torque is a very simple one. The main component is a magnetic sphere with radius $R_0 = 2 * 10^{-6}[m]$ and a magnetic moment $M = 1[T]$ pointing along the x-axis. Using the magnetic fields package it is possible to just define the magnetic moment to be along any direction. This magnetic particle is kept static while a magnetic field $H = 5 * 10^5[\frac{A}{m}]$ is applied, this field rotates along the y-axis which will result in

a torque along this axis. For the theoretical torque this magnetic field is assumed to be uniform and constant. However, as was proved in the previous section COMSOL actually does take into account the effects of the shape anisotropy, resulting in a non-uniform magnetic field inside of the particle. This can be seen clearly in figure 4.3, which shows three snapshots of the simulation for different angles of the magnetic field. The first image is taken when the magnetic field and magnetic moment are aligned, this would result in not magnetic torque. The magnetic field inside of the particle is less than outside, this is because of the demagnetisation field discussed in section 2.1.1. Using the parameters used in this model and equation 4.1 the maximum torque is calculated to be:

$$\begin{aligned}
 T_{max} &= V \tau = V M_s H \\
 &= \frac{4}{3} \pi R_0^3 M_s H \\
 &= \frac{4}{3} \pi (2 * 10^{-6} [m])^3 1 [T] 5 * 10^5 [\frac{A}{m}] \\
 &= 1.6755 * 10^{-11} [N m]
 \end{aligned} \tag{4.2}$$

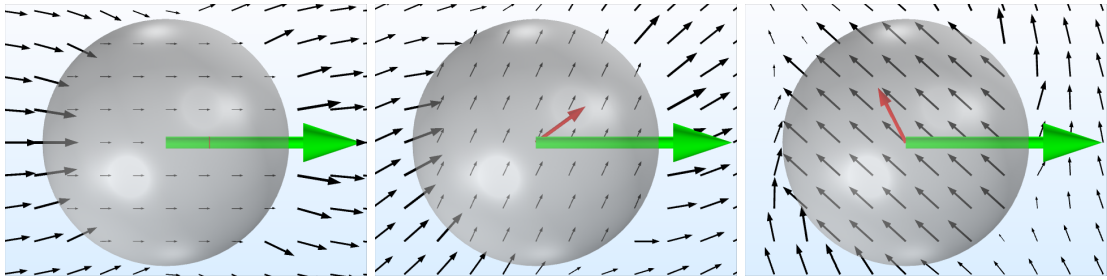


Figure 4.3: This series of figures shows the model used to verify the torque simulated by COMSOL. The spherical particle can be seen clearly in the middle of the figures. The green arrow represents the magnetic moment of the particle, the red arrows shows the angle of the applied magnetic field and the black arrows show the magnetic field lines simulated by COMSOL.

Figure 4.4 shows the results obtained from the COMSOL simulation. The dotted lines near the top and bottom of the graph show the theoretical value for the maximum torque calculated above. It is clear that the simulated torque does not reach the maximum theoretical value, this most likely is because the theoretical value assumes a uniform magnetic field. The conclusion of this verification is that the torque simulated by COMSOL is most likely a more accurate representation of the theoretical value used as a verification. This means that in future models, this torque can be used in the interaction of the particle with for instance a liquid or the membrane of cells.

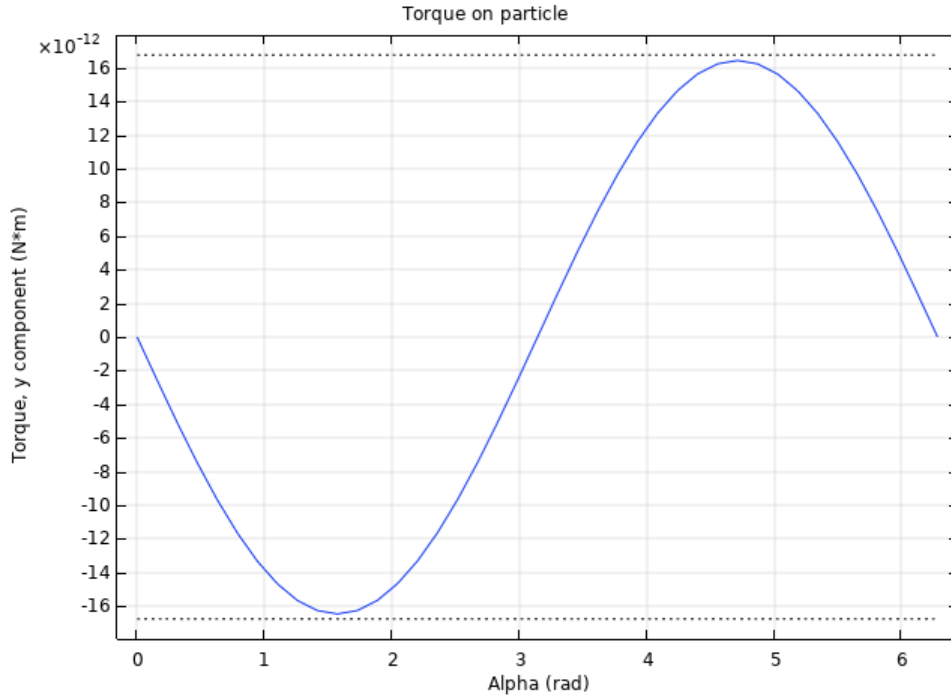


Figure 4.4: This graph shows the simulated torque using the COMSOL package, while the dotted line shows the theoretical maximum torque. For this model the torque on a spherical magnetic particle in a rotating magnetic field is simulated.

4.2 Model

To model all the different physics associated with the NanoPlatelets multiple packages will be used. First of all, as mentioned before, the magnetic fields package. This package will be used to simulate the physics between the external applied field and the static magnetic moments. Besides the magnetic field mechanics, this package can also be used to calculate the mechanical torque induced by the magnetic moment and field.

4.2.1 Geometry

The geometry used in this model can be described by three discs stacked upon each other, a figure of these discs can be found in the appendix A.1. The top and bottom discs are the cobalt discs and will be used for the magnetisation. The intermediate layers is ruthenium and is added for the simulation of the internal magnetic field. Since a big influence on the computation time used to solve the simulation is the meshing of the geometry, it is important to not only define the correct geometry but also use an appropriate finite element model. Since the diameter of the discs used in Mansell are $2\mu\text{m}$ while the thickness is on the order of a few nanometres, the meshing can be quite difficult. Because of some problems that arise with such a large difference in the geometry, the particle used in the model is only $0.2\mu\text{m}$. This effects the torque and the demagnetisation field.

4.2.2 Implementation of the Stoner-Wohlfarth model

The addition of the Zeeman interaction, anisotropy and the RKKY interaction proved to be more challenging than expected. Multiple solutions have been tried, but eventually the most practical solution has been to use a different package provided by COMSOL. This package is the weak

form partial differential equations package. This package solves any equation in the form of $u_t + u_x + u_y + u_z + u - f = 0$. Even though the Stoner-Wohlfarth model actually isn't a partial differential equation, it can be rewritten in a way that allows for the PDE package to solve for the minimum energy state. The target form for this rewritten equation is simply in the form $u = 0$, since it is not required for the PDE package to have differential (u_t, u_x, u_y, u_z) components. Of course $u = 0$ is a very basic equation, however there didn't seem to be a clear simple way of solving these kind of equations, which is why a partial differential equations package was used instead.

The challenging part of rewriting equation 2.14 is to realise that the minimum energy state is not the same as the zero energy state. Which is what would be solved for if equation 2.14 is simply be implemented without modifications in the PDE package. The minimum energy state is acquired by differentiating with respect to the angle θ , however there is no clear method of using the PDE package for this as it was just able to do spatial differentiation. It is still possible to use equation 2.14 to create a new equation such that:

$$u_{total}[\theta_1, \theta_2] - u_{Zeeman,target} - u_{Anisotropy,target} - u_{RKKY,target} = 0. \quad (4.3)$$

Here $u_{total}[\theta_1, \theta_2]$ is the original equation, with the dependent variables θ_1 and θ_2 . These variables represent the magnetic moment of the top and bottom layer. The three additions $u_{...,target}$ are the theoretical minima for each component of u_{total} . Equation 4.3 will only ever equal zero in absence of an applied magnetic field and with the magnetic moments aligned with the easy axis. When a magnetic field is applied, the PDE package will calculate a value for u_{total} using the dependent variables that approaches equation 4.3 as close as possible. To not get lost in the different formulas, the PDE package will solve the equation separate for the top and bottom layers, with the exception of the RKKY coupling of course. As discussed in the theory, the Zeeman and anisotropy energy are independent for each layer, simplifying the equations. In the next part, the different minima ($u_{...,target}$) used in equation 4.3 will be derived.

Starting with the Zeeman interaction, this term reaches the minimum energy when the magnetic moment and the magnetic field are aligned, or

$$\alpha - \theta = \Delta\phi = 0[rad]$$

the difference in angle between \vec{H} and \vec{M} . As described in section 2.1.2, the Zeeman interaction is based on the dot product between the magnetic moment and the magnetic field. This results in the following equation:

$$\begin{aligned} u_{Zeeman,target} &= -\vec{H} \cdot \vec{M} \\ &= -H M_s \cos(\Delta\phi) \\ &= -H M_s. \end{aligned} \quad (4.4)$$

As discussed in the theory, the anisotropy energy can only every be zero or positive. This implies that this term is already in the desired form

$$K \sin(\theta_i)^2 = 0.$$

Here the subscript i indicates the different layers, $i = 1$ for the top layer and $i = 2$ for the bottom layer. Therefore, $u_{Anisotropy,target} = 0$.

Because for NanoPlatelets $J > 0$, the RKKY energy is only minimal when the magnetic moments of the top and bottom layer are aligned anti-parallel ($\theta_1 - \theta_2 = \pm\pi[rad]$). This results in

$$\begin{aligned}
 u_{RKKY,target} &= \frac{J}{t} \cos(\theta_1 - \theta_2) \\
 &= \frac{J}{t} \cos(\pm\pi) \\
 &= -\frac{J}{t}.
 \end{aligned} \tag{4.5}$$

However, taking the dependent variables to be θ_i turned out to be incorrect. These angles can be any value between 0 and 2π , and it would wrap around from 2π back to 0. The wrapping around is not something that COMSOL recognises, and because of the way it solves the problem it resulted in values for θ_i in the thousands radians. A solution to this problem is to use different dependent variables, which are not angles. For this model the different vector components, M_x M_y M_z , of the magnetic moments are used, instead of the angle of these vectors. The downside of using the vector components as opposed to the angle, is that the length of the vector is not static anymore. To solve this problem a point-wise constraint (part of the PDE package) is added, which will require $\text{sqr}t(M_x^2 + M_y^2 + M_z^2) = M_s$ to always be true. This change of dependent variables results in an equation with six dependent variables (three for each magnetic layer) as opposed to two dependent variables (one for each magnetic layer).

Changing from an angle to the vector component requires some other adaptations besides the constraint of the vector length. The dot and cross product used in equation 2.14 need to be rewritten as well. The RKKY interaction can also be rewritten to be a normalised dot product, rewriting the cosine using

$$\cos(\Delta\phi) = \left(\frac{\vec{M}_1 \cdot \vec{M}_2}{M_s^2} \right).$$

COMSOL then solves equation 4.3 and tries to approach a solution of

$$u_{total}[M_{1,x}, M_{1,y}, M_{1,z}, M_{2,x}, M_{2,y}, M_{2,z}] - u_{total,target} = 0$$

as closely as possible, such that the different weights (H M_s , K , $\frac{J}{t}$) of the energy function determine their impact on the final solution.

4.2.3 Shape anisotropy

The reason for chapter 4.1.1 is of course to investigate if K can be used as opposed to K_{eff} . So the different parameters used in the PDE should be acquired from the simulation itself. Of course this means that the resulting magnetic field is dependent on the orientation of the magnetic moments, which in turn is dependent on the internal magnetic field. This is where the solver comes into play, COMSOL can solve the physics in a manner that makes them coupled, or solves them independently and then combines them afterwards. Both have their pros and cons, for this problem and because it was found that using a different solver configuration for the magnetic fields package as opposed to the PDE package the segregated solver is used. Which first solves for the magnetic fields lines, after which it passes the \vec{H} and \vec{M} components to the PDE package which uses these components to solve for $M_{i,j}$ for $i = 1, 2$ and $j = x, y, z$. These components are then used to define the magnetisation using the magnetic fields package.

4.2.4 Solver

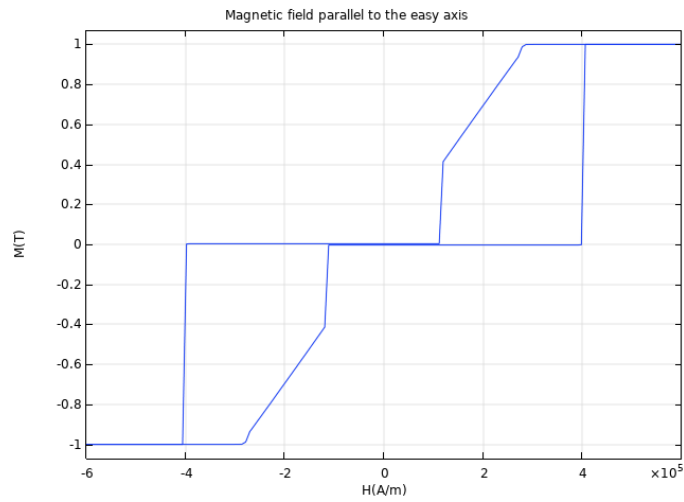
As mentioned above, the solver used is a segregated one. Besides this there also is an added parametric sweep, this is the part of the solver that changes one or more parameters in the model and then runs the solver for this new situation. The model right now just changes the strength of the magnetic field based on the increments and range set manually. Thanks to delving into the settings associated with the parametric sweep, found under the parametric solver, an option is enabled to start the new simulation given the solution from the previous solver iteration.

4.3 Results

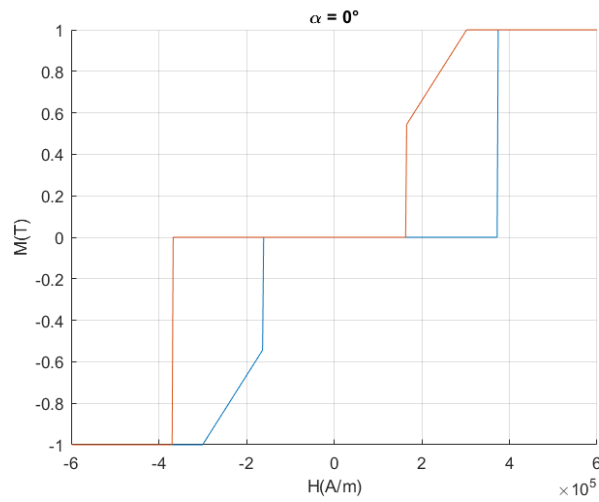
In this section the results obtained from the running the simulation in different configurations are discussed, these configurations are identical to the ones used in the MatLab model (section 3.1). Similarly the parameters used for this simulation are: $M_s = 1[T]$, $K = 1.03 * 10^5 [\frac{J}{m^3}]$, $J = 2.5 * 10^{-4} [\frac{J}{m^2}]$ and $t = 9 * 10^{-10} [m]$, again equal to the parameters used in the MatLab model. In these simulations, the magnetic field is varied from $H = -6 * 10^5 [\frac{A}{m}]$ to $H = +6 * 10^5 [\frac{A}{m}]$. The parameter describing the angle of the magnetic field with respect to the particle is the θ parameter, as opposed to the α parameter used for the MatLab model. The first situation simulated is when the magnetic field is parallel to the easy axis, and thus $\theta = 0[rad]$. As discussed in section 3.1 the total magnetic moment is expected to be zero, as the individual moments are aligned anti-parallel. For the extreme values of the magnetic field strength, these magnetic moments will be aligned with the applied magnetic field. The results of this simulation can be seen in figure 4.5a. To be able to make a comparison with the results obtained by the MatLab model the graph from the MatLab simulation is shown underneath it.

Figure 4.5 allows for the comparison of the two models, and as a result allows something to be said about the viability of modelling the magnetic behaviour of NanoPlatelets using COMSOL. The first check would be to see if the COMSOL model is in agreement with the assumptions made before about the behaviour. These being the net zero total magnetisation when the external magnetic field is absent. As well as the magnetisation reaching the saturation magnetisation for strong magnetic fields. These two main assumptions are indeed present in the simulation results of COMSOL. There are a few deviations between the results obtained using the MatLab model and the COMSOL model.

The first anomaly occurs around $H = \pm 4 * 10^5 [A/m]$, the MatLab model predicts that the switch happens slightly earlier, around $H = \pm 3.7 * 10^5 [A/m]$.



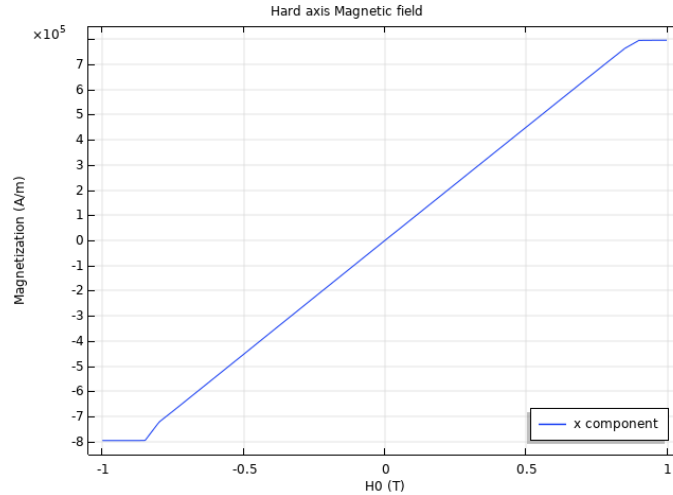
(a) Graph showing the magnetisation as simulated by COMSOL, the effect of the shape anisotropy is calculated by COMSOL.



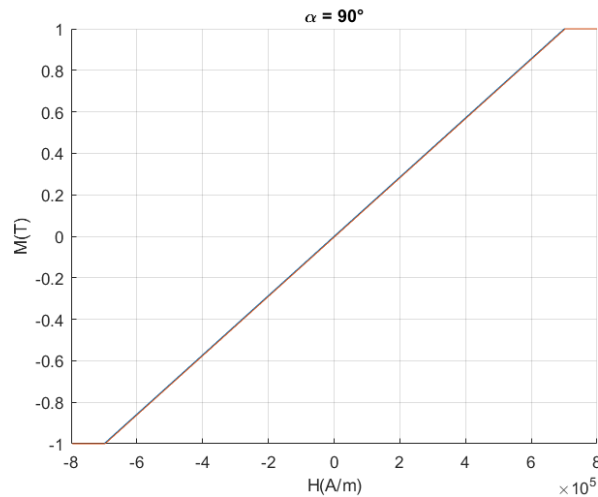
(b) Graph showing the magnetisation as simulated by MatLab, here K_{eff} is approximated using equation 2.6

Figure 4.5: Shown here are the results for running the simulations with the magnetic field parallel with the easy axis. Both models used the same parameters, with the exception of K_{eff} .

The next configuration of the simulation is for when the magnetic field is perpendicular to the easy axis. However, unlike with the 3D model, there is not just one direction that is perpendicular to this axis. Because of this the magnetic field is defined to be laying along the x-axis, resulting in just the x-component of the magnetisation changing. This is why in figure 4.6 the only part shown is the x-component of the total magnetisation.



(a) Graph showing the magnetisation as simulated by COMSOL, the effect of the shape anisotropy is calculated by COMSOL. Because of a mistake, the magnetic field along the x-axis is plotted using the unit of T as opposed to the unit A/m . Similarly the y-axis shows the magnetisation using A/m as opposed to T .

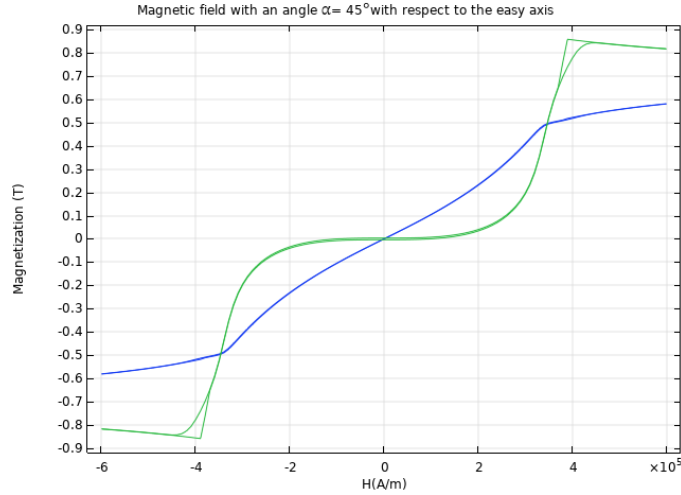


(b) Graph showing the magnetisation as simulated by MatLab, here K_{eff} is approximated using equation 2.6

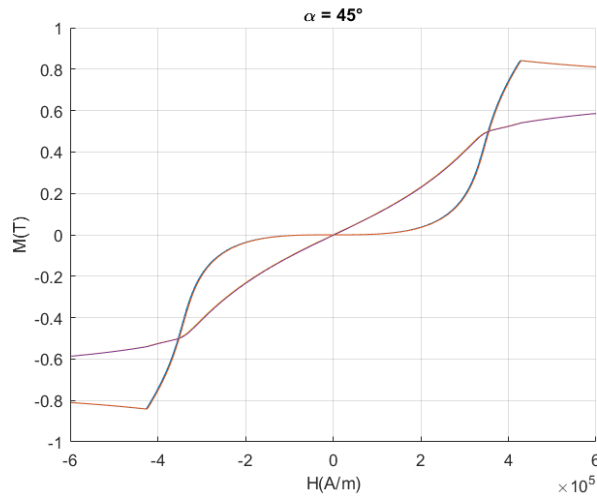
Figure 4.6: Shown here are the results for running the simulations with the magnetic field having an angle of $\alpha = 90^\circ$ with the easy axis. Both models used the same parameters, with the exception of K_{eff} .

The results shown in this figure are because of the difference in units used not comparable. However the shape of the graph does agree with the expectations.

The last configuration used to compare the COMSOL model to the MatLab model is for a magnetic field diagonal to the easy axis. The results can be seen in figure 4.7a.



(a) Graph showing the magnetisation as simulated by COMSOL, the effect of the shape anisotropy is calculated by COMSOL.



(b) Graph showing the magnetisation as simulated by MatLab, here K_{eff} is approximated using equation 2.6

Figure 4.7: Shown here are the results for running the simulations with the magnetic field having an angle of $\alpha = 45^\circ$ with the easy axis. Both models used the same parameters, with the exception of K_{eff} .

Similar to the other simulations, the MatLab model and COMSOL model agree on most points. For this simulation a slight difference can be seen near $H = \pm 4 \times 10^5 [\frac{A}{m}]$. This implies that the magnetisation prefers the local energy minimum more in the COMSOL model than it does for the MatLab model. This can very well be a result from the settings used for the PDE package, or the COMSOL solver in general.

Chapter 5

Conclusions

COMSOL multiphysics is a program used in creating models using many different physics, therefore it could be useful in modelling NanoPlatelets. However, the magnetic fields package provided by COMSOL only simulates the behaviour of permanent magnets, which is not useful for describing the NanoPlatelets. The Stoner-Wohlfarth model does predict the more complex behaviour associated with the NanoPlatelets. The aim of this thesis has been to implement the Stoner-Wohlfarth model in COMSOL. A MatLab script was written to provide a tool to verify the results obtained using COMSOL.

Part of this process has been the verification of the demagnetisation field and magnetic torque simulate by COMSOL. The simulation results are compared with results obtained from the MatLab model. the comparison resulted in a few deviations between the results. The three main reasons for these deviations are:

- The COMSOL model uses the simulated demagnetisation field, based on the geometry of the particle, to include the shape anisotropy used in the Stoner-Wohlfarth model. The MatLab model however uses an approximation for this, assuming the particle to be an infinite wide plane.
- The COMSOL model is three dimensional, while the MatLab model is only two dimensional. This provides an additional degree of freedom for the magnetic moments of the NanoPlatelet.
- As with any simulation, COMSOL has numerical inaccuracies. These are mentioned here because depending on the solver setting used the error can be decreased at the cost of computation time.

5.1 Outlook

The first reason mentioned for the deviations between the MatLab model and the COMSOL model is the shape anisotropy of the particle. This shape anisotropy is caused by the demagnetisation field and it has been verified that COMSOL correctly calculates these fields. However, the Stoner-Wohlfarth model uses an approximation for this shape anisotropy. COMSOL could be used to refine this approximation by calculating the shape anisotropy of the NanoPlatelet. The calculated anisotropy can then be used in the MatLab model to provide a more accurate verification.

Both the COMSOL model and the MatLab model assume top and bottom layer are equal, both in thickness as in their magnetic moment. It might be interesting to investigate the effects of creating an imbalance between the two layers, by either changing the magnetic moment or the thickness of the magnetic layer. This imbalance would result in a anti-ferrimagnetic particle, as opposed to an anti-ferromagnetic particle.

Besides for the verification of the simulated torque, the force calculation of COMSOL has not been used.

The reason for using COMSOL is to be able to create a model for the interaction of NanoPlatelets with the membrane of cancer cells. Such a model would need to include some fluid dynamics, to simulate what happens when the NanoPlatelets enter the blood stream for instance. Since fluid dynamics on the nano-scale could be a thesis all on its own, this has not been investigated. However, some progress has been made towards this final goal. This has resulted in being able to create a particle that is able to freely rotate, using a specific meshing technique called a moving mesh. Future research could couple this rotation with the magnetic torque of the particle.

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Appendix A

Double domain Stoner-Wohlfarth model

```

close all
clear

%Define in how many steps the model gets calculated, MaxH is the amount
%centered around H=0
MaxH=30000;
Steps=2000;
dStep=MaxH/Steps;

%Initialise constants, for simplicity they are combined into an array
Ms=900;
J=0.25;
%K=2.66*10^6;
t=0.9E-7;
Hk=5000;
K=Hk*Ms/2;

Constant=[Ms,K,J,t];

%Random disturbance to check if the current minimum is not just a turning
%point
Disturb=[0,0];

%Define function
E = @(x,H,a,Constant) -H*Constant(1)*(cos(a-x(1))+cos(a-x(2)))+Constant(2)*(sin(x(1)).^2+sin(x(2)).^2)+Constant(3)*cos(x(1)-x(2))/(Constant(4));

%Start plots
x1Per=subplot(2,2,1);
hold(x1Per,'on')
x2Per=subplot(2,2,2);
hold(x2Per,'on')
x1Parallel=subplot(2,2,3);
hold(x1Parallel,'on')
x2Parallel=subplot(2,2,4);
hold(x2Parallel,'on')

for j=0:90:0
    a=deg2rad(j);

    minimum=zeros([Steps 2 2]);
    Energy=zeros(Steps,2);
    Torque=zeros(Steps,2);
    Prev=[0,pi];
    options = optimset('MaxFunEvals', 1000*2);

    for i=1:Steps
        %This for loop goes from -MaxH/2 to +MaxH/2
        H=i*dStep-MaxH/2;

        [minimum(i,:,1),Energy(i)] = fminsearch(@(x) E(x,H,a,Constant),Prev);

        Disturb=[0.01*(rand-0.5),0.01*(rand-0.5)];
        Prev=minimum(i,:,1)+Disturb;
    end

    for i=1:Steps
        %This for loop goes from +MaxH/2 to -MaxH/2

```

```

H=-i*dStep+MaxH/2;
p=Steps+1-i;

[minimum(p,:,2),Energy(p)] = fminsearch(@(x) E(x,H,a,Constant),Prev);

Disturb=[0.01*(rand-0.5),0.01*(rand-0.5)];
Prev=minimum(p,:,2)+Disturb;
end

normEnergy=Energy./max(abs(Energy));

%Since for a=0 both angles x(1) and x(2) are 0/2pi the wrap command
%gets confused, to alleviate this I introduce an offset which I then add
%again after the wrapping
minimum=wrapToPi(minimum-0.5*pi);
minimum=minimum+0.5*pi;

%Define the perpendicular moment(with regard to the EA) and the
%parallel component
mPerp=sin(minimum);
mParallel=cos(minimum);

Angle=string(j)+' Degree';

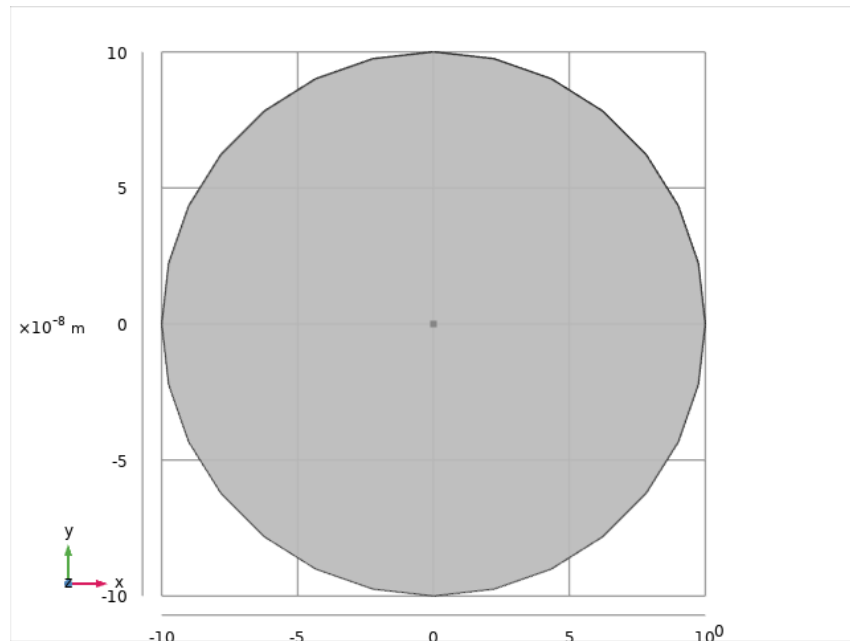
plot(x1Per,dStep*(1:Steps)-MaxH/2,mPerp(:,1,1))
plot(x1Per,dStep*(1:Steps)-MaxH/2,mPerp(:,1,2))
plot(x2Per,dStep*(1:Steps)-MaxH/2,mPerp(:,2,1))
plot(x2Per,dStep*(1:Steps)-MaxH/2,mPerp(:,2,2))
plot(x1Parallel,dStep*(1:Steps)-MaxH/2,mParallel(:,1,1))
plot(x1Parallel,dStep*(1:Steps)-MaxH/2,mParallel(:,1,2))
plot(x2Parallel,dStep*(1:Steps)-MaxH/2,mParallel(:,2,1))
plot(x2Parallel,dStep*(1:Steps)-MaxH/2,mParallel(:,2,2))

end

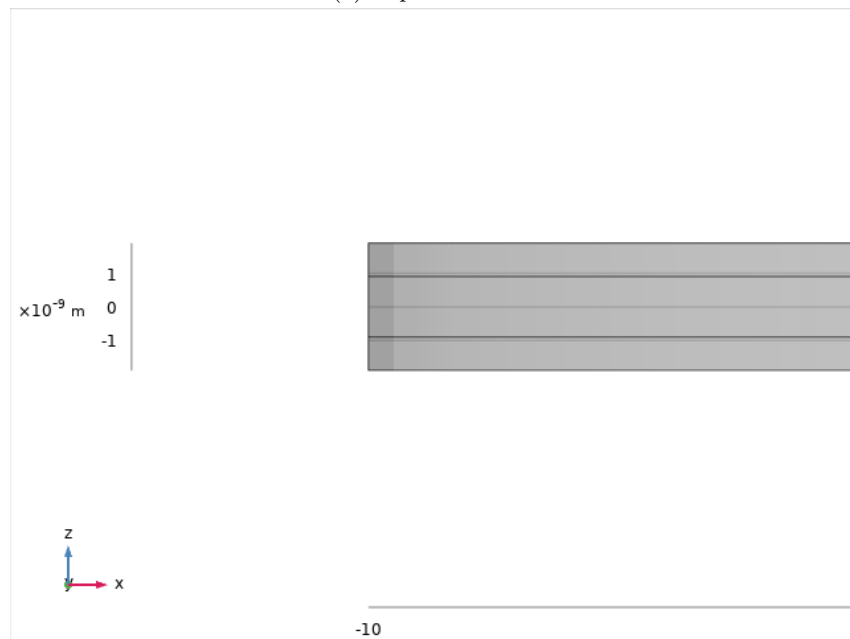
title(x1Per,'Perpendicular component magnetic moment, x1')
title(x1Parallel,'Parallel component magnetic moment, x1')
title(x2Per,'Perpendicular component magnetic moment, x2')
title(x2Parallel,'Parallel component magnetic moment, x2')

hold(x1Per,'off')
hold(x1Parallel,'off')
hold(x2Per,'off')
hold(x2Parallel,'off')

```



(a) Top-down view



(b) Side view

Figure A.1: In this figure the geometry used in the COMSOL model is presented. As can be seen from the figures and has been discussed in section 4.2.1 the geometry consists out of three discs on top of each other. The top and bottom layer represent the magnetic layers, and the intermediate disc represents the non-magnetic spacer layer.