

Imperial College London
Department of Earth Science and Engineering

Nine month report

Miguel A. Valdez Grijalva

Submitted in compliance with the requirements of a Research PhD programme,
Imperial College London, October 2014

Abstract

It is known from aeromagnetic surveys from Venezuela, China and the U.S.A. that it is common to find geomagnetic anomalies over oil fields. It has been suggested that hydrocarbon reservoirs, through upward seepage, create physical and geochemical conditions in soils and rocks sitting above them that are conducive to the formation of secondary ferrimagnetic minerals such as magnetite and greigite. In near-surface samples drilled in Venezuela it has been observed that these minerals form aggregates of roughly spherical grains called *framboids*. While the specific physical and geochemical processes involved in the genesis of these minerals is an active research topic, I will focus in studying the domain structure and hysteresis parameters of these minerals via numerical simulation of the *micromagnetic* equations. Solving the micromagnetic problem can be done either by minimising the total Gibbs free energy which is a sum of energies associated with different phenomena in a ferromagnetic material or by solving the dynamical equation for the magnetic moments, that is, the Landau-Lifshitz-Gilbert equation (LLGE). I will use a finite element method based on the general-purpose package collection for automated solutions of partial differential equations *FEniCS* to solve the LLGE as well as an energy minimising routine, specifically a conjugate gradient method. My aim is to find the magnetic response of these mineral aggregates measured in a given sample by standard rock-magnetic and palaeomagnetic techniques. As a first approach to the problem, before scaling up the simulations, I have conducted simulations of hysteresis loops and zero-field domain structure of octahedral-shaped single grains of greigite and compared these with octahedral grains whose corners have been chopped. These shapes are typical morphologies of greigite and so, these simulations constitute an improvement over previous finite difference models that could only study somewhat unrealistic shapes like cubes and rectangular prisms.

Contents

Abstract	i
1 Introduction	1
1.1 Motivation and Objectives	1
2 Background theory	4
2.1 Magnetism and matter	4
2.1.1 Fundamentals of magnetism	4
2.1.2 Diamagnetism and paramagnetism	6
2.1.3 Ferromagnetism	7
2.1.4 Magnetic Gibbs free energy	8
2.1.5 The Landau-Lifshitz-Gilbert equation	11
2.1.6 Micromagnetic modelling	11
3 Results	14
4 Plan	15
Bibliography	15

Chapter 1

Introduction

1.1 Motivation and Objectives

It has been established via airborne magnetic surveys in the U.S.A. (Donovan et al., 1979) that magnetic contrasts—that is, “magnetisation that is different from background magnetisation and which may give rise to mappable magnetic anomalies detectable by conventional magnetometry” (Machel and Burton, 1991)—are a common feature of hydrocarbon reservoir sites. Donovan et al. (1979) suggested that these magnetic anomalies are caused by near-surface magnetic minerals (specifically, magnetite) induced by upward hydrocarbon seepage from the underlying hydrocarbon reservoir. Further studies by Donovan et al. (1984), Reynolds et al. (1993) and Elmore et al. (1993) in the U.S.A., Díaz et al. (2000), Costanzo-Alvarez et al. (2006), Guzmán et al. (2011), González et al. (2002) in Venezuela and Liu and Liu (1999), Liu et al. (2004) and Liu et al. (2006) in China have provided strong evidence for a genetic relationship between the magnetic contrasts produced by ferrimagnetic minerals near the surface and the underlying reservoir. These investigations confirm the original hypothesis of Donovan et al. (1979) that the reducing environment caused by the upward seepage from the reservoirs is conducive to the formation of magnetic minerals—such as magnetite and other Fe-oxides, and greigite and other Fe-sulfides—and/or the destruction of minerals such as hematite (Machel and Burton, 1991) and thus further the case for using a combination of aeromagnetic surveying and

rock-magnetic measurements of soils and rocks for cheap hydrocarbon prospecting as proposed by Donovan et al. (1984).

Though the discussion on the exact mechanism for the formation of these minerals is ongoing, Machel and Burton (1991) have identified two primary agents for the precipitation of magnetic minerals under the influence of hydrocarbon seepage. At higher temperatures and thus higher depths they propose chemical processes as the main factor while at shallower depths and lower temperatures it is argued that microbial sulfate-reducing processes are playing the larger role. Machel and Burton (1991) also emphasised the difficulty in linking a magnetic anomaly to a process of hydrocarbon seepage because the precipitation of magnetic minerals can cause positive or negative anomalies—that is, peaks or dips in the geomagnetic field and/or the magnetic susceptibility of the soils. Nevertheless, careful analysis of the local conditions can result in the successful application of rock-magnetic measurements to hydrocarbon exploration (see Liu et al. (2006) and Donovan et al. (1984)). Magnetization of oil bearing rocks can also be used to assess the quality of oil as discussed by Emmerton et al. (2013).

It was recognized by Reynolds et al. (1993) that in some cases iron sulfides may be more important to the magnetic contrasts and thus to the identification of prospective oil-producing fields than iron oxides. Particularly, greigite has been identified as an authigenic mineral of the utmost importance in the Simpson oil field in Alaska (Reynolds et al., 1993). Greigite is an iron sulfide (Fe_3S_4) that can be thought of as the sulfur equivalent of the iron oxide magnetite (Fe_3O_4) as they have the same crystal structure only with sulfur replacing oxygen. Like magnetite, it is highly magnetic. Nevertheless, since it is thought to be unstable, its importance as a palaeomagnetic recorder has not been as readily realized as that of magnetite. Also, its magnetic parameters were poorly understood until the work of Chang et al. (2008) who by synthesising highly pure greigite were able to measure the critical magnetic parameters. Muxworthy et al. (2013) made use of the new accurate measurements of greigite to simulate greigite grains and the effect of intergrain interactions.

Liu et al. (2006) has proposed that magnetic mineral grains that are linked to hydrocarbon seepage have sizes $\sim 25\text{nm}$ and thus generally in the single domain (SD) range. In terms of

morphology, it has been repeatedly found (see Aldana et al. (1999) and references therein) that roughly spherical grains of magnetite and/or greigite assemble in raspberry-shaped aggregates called framboids (from the french *framboise* meaning raspberry). It is my interest to model these structures via micromagnetics to investigate their domain structure and behaviour in routine rock-magnetic and palaeomagnetic measurements that could also correlate with the size of the aggregates. It is an open question how the intergrain interactions will affect the otherwise simpler problem of modelling single grains, however Muxworthy et al. (2003), Muxworthy et al. (2013) have made a strong case for the importance of intergrain magnetostatic interactions. Further understanding of framboidal aggregates of greigite or magnetite could aid in developing future oil exploration techniques that are cheaper than more conventional techniques vastly used today.

Chapter 2

Background theory

2.1 Magnetism and matter

2.1.1 Fundamentals of magnetism

The magnetic field, just like the electric field, is defined by the its effect on a *test charge*, namely the Lorentz force:

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B} , \quad (2.1)$$

where q is the electrical charge, \mathbf{v} its velocity and \mathbf{E} and \mathbf{B} the electrical and magnetic field (although for historical reasons \mathbf{B} is called the *induction* field). Clearly the force a magnetic field exerts on a moving electrical charge is perpendicular to both its velocity and to the field itself. From the Lorentz law it is readily seen that the unit of \mathbf{B} is $\frac{\text{N}}{\text{C} \cdot \frac{\text{m}}{\text{s}}}$, this physically meaningful unit is called Tesla, with symbol T.

The description of magnetic fields is analogue to that of electrical fields. Although, unlike the situation in electricity, there are no magnetic charges, only magnetic dipoles. A more thorough analysis reveals the origin of magnetism is electrical: an electrical current (either a flow of electrons or a single electron) produces an induction field \mathbf{B} . The induction due to a wire carrying a current I (generally varying along the path) at point \mathbf{r} can be calculated from the

Biot-Savart law:

$$\mathbf{B}(\mathbf{r}) = \frac{\mu_0}{4\pi} \int_C \frac{I d\mathbf{l} \times \mathbf{r}}{r^3}, \quad (2.2)$$

where $d\mathbf{l}$ is a differential element of length along the wire in the direction of the current. The integral is carried out along a line, usually but not necessarily a closed curve. Thus, on a fundamental level it is correct to understand magnetism as an electrical phenomenon.

When describing magnetic fields the *magnetic induction* \mathbf{B} and the *magnetic field* \mathbf{H} are used. These denominations are of historical character and it has been proven that the true fundamental field is the induction field \mathbf{B} (for a thorough discussion of why this is so see Feynman et al. (1964)) while \mathbf{H} represents contributions to the field by macroscopic currents. Other contributions to the magnetic field are due to atomic dipoles and circular currents in a medium. In a vacuum, \mathbf{B} and \mathbf{H} coincide in direction as there are no atomic magnetic dipoles present. In the SI the magnetic and induction field differ by a scalar factor μ_0 , the *magnetic constant*, also known as the vacuum permeability or permeability of free space:

$$\mu_0 = \frac{B_{vacuum}}{H} = 4\pi \cdot 10^{-7} \frac{\text{V} \cdot \text{s}}{\text{A} \cdot \text{m}}. \quad (2.3)$$

Although the names vacuum permeability and permeability of free space are still widespread it is preferable to use the name magnetic constant since it reflects the fact that it's a defined value and not a measurement.

In general, we are not interested in describing magnetic phenomena in a vacuum, rather it is more interesting and important to consider the presence of matter. A material is composed of atoms, which individually may hold a permanent magnetic dipole moment μ (with units $\text{A} \cdot \text{m}^2$). The *magnetisation* vector field \mathbf{M} is the spatial average of a myriad of these individual atomic dipole moments over a suitable volume. Therefore, \mathbf{M} accounts for the contribution of atomic magnetic moments to the total field. In the SI units we have

$$\mathbf{B} = \mu_0(\mathbf{H} + \mathbf{M}); \quad (2.4)$$

immediately we see that both \mathbf{H} and \mathbf{M} have the same units, the Ampere per meter $\frac{\text{A}}{\text{m}}$.

Mineral	Magnetic susceptibility (per unit mass)
	($10^{-8}\text{m}^3/\text{kg}$)
<i>Diamagnetic</i>	
Quartz (SiO_2)	-0.62
Orthoclase feldspar (KAlSi_3O_8)	-0.58
Calcite (CaCO_3)	-0.48
Forsterite (Mg_2SiO_4)	-0.39
Water (H_2O)	-0.90
<i>Paramagnetic</i>	
Pyrite (FeS_2)	30
Siderite (FeCO_3)	123
Ilmenite (FeTiO_3)	100–113
Orthopyroxenes ($(\text{Fe,Mg})\text{SiO}_3$)	43–92
Fayalite (Fe_2SiO_4)	126
Intermediate olivine ($(\text{Fe,Mg})_2\text{SiO}_4$)	36
Serpentine ($\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_4$)	≥ 120
Amphiboles	16–94
Biotites	67–98
Illite (clay)	15
Montmorillonite (clay)	14

Table 2.1: Magnetic susceptibilities of diamagnetic and paramagnetic materials. Reproduced from Dunlop and Özdemir (1997).

2.1.2 Diamagnetism and paramagnetism

Magnetism in matter can be broadly categorised into three phenomena: diamagnetism, paramagnetism and ferromagnetism. Diamagnetism and paramagnetism are of little importance to us so we will only briefly describe them.

Diamagnetism is a property of all matter. It is the smallest effect and is a tendency of a material to oppose an external magnetic field. An external magnetic field exerts a Lorentz force on the bound electrons that causes them to precess like a gyroscope. This is called Larmor precession and is equivalent to an electric current producing a magnetic moment in the direction opposed to the external \mathbf{B} field. Water is a common example of a highly diamagnetic material.

Paramagnetism is a partial alignment of the permanent atomic magnetic moments of the atoms in a material with an external \mathbf{B} field. It is only thermal noise that prevents a perfect alignment of the atomic magnetic moments with the external field, therefore this is a highly temperature dependent phenomenon. Nevertheless, at ordinary temperatures, paramagnetism outweighs

diamagnetism by a factor greater than 10.

In both diamagnetism and paramagnetism a magnetisation is induced by an external field. The rate at which the magnetisation is acquired with respect to the applied field is called the *magnetic susceptibility* $\chi = \frac{d\mathbf{M}}{d\mathbf{H}}$, in general a tensor. Table 2.1.2 (reproduced from Dunlop and Özdemir (1997)) lists susceptibility values for some diamagnetic and paramagnetic materials.

2.1.3 Ferromagnetism

A common theme in diamagnetism and paramagnetism is that an external field induces a temporary magnetisation in the material; once the external field is removed the material loses its magnetisation. Also, at ordinary temperatures, only extremely high external fields of the order of 100 Tesla (for a sense of scale, the Earth's magnetic field is of the order of 10^{-4}T) can induce in a paramagnetic material a saturation magnetisation—that is, a magnetisation that results from all the atomic magnetic moments aligning in exactly the same direction. A ferromagnetic material like Iron or Nickel is fundamentally different in both these aspects. It only takes external fields of the order of 0.1 Tesla to achieve a saturation magnetisation M_s and once the external field is suppressed the ferromagnetic material holds a measurable remanent magnetisation M_r .

Ultimately, ferromagnetism is a phenomenon that cannot be explained solely by classical physics. At the core is the quantum-mechanical concept of *spin exchange coupling*, a phenomenon with no classical counterpart. It was in Landau and Lifshitz (1935) that a continuum expression for the exchange energy was obtained. This seminal work and that of W. F. Brown (1940) are the theoretical basis from which micromagnetism emerged. Micromagnetism is a theory that bridges the fundamental quantum-mechanical picture and the effective macroscopic theory of Maxwell equations. Therefore it operates in a scale that is sufficiently large to contain hundreds of atoms making it possible to think of the material as a continuum but not large enough to be described by the effective theory of Maxwell equations. The main goal of a micromagnetic investigation is to obtain a configuration of the magnetic moments in a ferromagnetic material. The main result in Landau and Lifshitz (1935) was the theoretical proof that inside

a ferromagnetic material there are regions that are magnetised to saturation called magnetic *domains* and that between these domains exist regions where the magnetisation continuously rotates from the direction of one domain to that of the other, these are called *domain walls*.

There are two main approaches to micromagnetism. One is obtaining a configuration of the magnetic moments in a ferromagnetic material by minimising the magnetic Gibbs free energy. The other is to solve a partial differential equation that describes the actual dynamics of the magnetic moments; this equation was derived by Landau and Lifshitz (1935) and improved by Gilbert, so it's appropriately called the Landau-Lifshitz-Gilbert equation (LLGE).

2.1.4 Magnetic Gibbs free energy

Magnetic energy is that which is dependent on the magnetisation of the material. It is known from thermodynamics that starting from a nonequilibrium state the evolution of a system can be only such that its Gibbs free energy diminishes. So, by an explicit formulation of the different energies contributing to the total magnetic Gibbs free energy it is possible to find a configuration that is either a local energy minimum (LEM) or global energy minimum (GEM). One of the biggest contributions of micromagnetics to our understanding of magnetic phenomena in matter is that it is quite common for a material to be in a LEM configuration rather than GEM. We will now briefly review four magnetic energies that contribute to the total. There are microscopic contributions like the exchange energy and the magnetocrystalline anisotropy energy. Also macroscopic contributions like the magnetostatic energy and the Zeeman energy. For simplicity we will not be interested at this moment in the magnetoelastic energy due to mechanical stress and deformation of the material. The external or Zeeman field is independent of the magnetisation and the exchange and anisotropy energies are short range so these are very easy to calculate. The magnetostatic interaction between the magnetic moments is a long range interaction and is the most numerically expensive contribution. This energy creates a demagnetising effect. Thus, we can write the total magnetic Gibbs free energy as

$$E_{\text{total}} = \int_{\Omega} (\omega_{\text{exch}} + \omega_{\text{anis}} + \omega_{\text{demag}} + \omega_{\text{zeeman}}) dv . \quad (2.5)$$

The exchange energy is a quantum-mechanical phenomenon wherein the exchange of inner shell electrons between neighbouring atoms results in the so-called spin exchange coupling. The continuum expression was obtained by Landau and Lifshitz (1935) and found to be proportional, up to a constant, to the square of the gradient of the magnetisation distribution:

$$\omega_{\text{exch}} = A \left((\nabla u_x)^2 + (\nabla u_y)^2 + (\nabla u_z)^2 \right), \quad (2.6)$$

where A is the exchange stiffness constant and $\mathbf{M} = M_s \mathbf{u}$, i.e., \mathbf{u} is a unit vector in the direction of the magnetisation. The effect of the exchange energy is that it homogenises the distribution of moments.

The magnetocrystalline anisotropy energy is due to the atomic configuration of a crystalline material. The specific arrangement of atoms in the crystal can cause some directions to be easier for the moments to align with. These directions are called *easy axis*. The anisotropy energy of a uniaxial system (one that has only one easy axis) is given by

$$\omega_{\text{anis}} = K_1 (1 - (\mathbf{a} \cdot \mathbf{u})^2), \quad (2.7)$$

where K_1 is the first anisotropy constant and \mathbf{a} is a unit vector in the direction of the easy axis. The effect of the anisotropy energy is a tendency for the magnetic moments to align with the easy axis of magnetisation.

The Zeeman energy is just the potential energy associated to the magnetic moments when an external or Zeeman field is applied.

$$\omega_{\text{zeeman}} = -\mathbf{M} \cdot \mathbf{B}_Z, \quad (2.8)$$

where \mathbf{B}_Z is an external magnetic induction field. This energy tends to align the magnetic moments with the external field.

The magnetostatic energy is due to the magnetostatic interaction each magnetic moment has with each other. Since in a micromagnetic model there can be hundreds of thousands of

individual magnetic moments it's the most expensive to calculate. Many methods have been devised to avoid calculating this interaction for each moment, most of these based on the magnetic vector or scalar potential. We refer to Abert et al. (2013) and Imhoff et al. (1990) for two such methods. The magnetostatic energy creates a demagnetising effect, that is, an internal field $\mathbf{B}_{\text{demag}} = \mu_0 \mathbf{H}_{\text{demag}}$ produced by the magnetisation distribution that opposes the magnetisation. It is also the phenomenon that has the biggest role in the domain structure of bigger materials. Once this demagnetising field is calculated, the magnetostatic energy can be expressed as

$$\omega_{\text{demag}} = -\frac{1}{2} \mathbf{M} \cdot \mathbf{B}_{\text{demag}}, \quad (2.9)$$

where the factor $\frac{1}{2}$ is added because the interaction of magnetic moment μ_i with μ_j is counted twice.

We may now rewrite equation (2.5) as

$$E_{\text{total}} = \int_{\Omega} \left(A ((\nabla u_x)^2 + (\nabla u_y)^2 + (\nabla u_z)^2) + K_1 (1 - (\mathbf{a} \cdot \mathbf{u})^2) - \mathbf{M} \cdot \mathbf{B}_Z - \frac{1}{2} \mathbf{M} \cdot \mathbf{B}_{\text{demag}} \right) dv. \quad (2.10)$$

A system out of equilibrium will evolve by diminishing its free energy. The aim of micromagnetic theory is to obtain a distribution of the magnetic moments in equilibrium. Brown (1963) proposed a variational method based on the variational derivative of the total energy with respect to the magnetisation. In equilibrium, the variation of the free energy vanishes

$$\frac{\delta E_{\text{total}}}{\delta \mathbf{u}} = 0. \quad (2.11)$$

This leads to Brown's equation

$$\mathbf{u} \times (2A\Delta \mathbf{u} + 2K_1 \mathbf{a}(\mathbf{u} \cdot \mathbf{a}) + M_s \mathbf{B}_Z + M_s \mathbf{B}_{\text{demag}}) = 0. \quad (2.12)$$

This means that in equilibrium the magnetisation is parallel to an *effective field*

$$\mathbf{B}_{\text{eff}} = \frac{2}{M_s} \Delta \mathbf{u} + \frac{2K_1}{M_s} \mathbf{a}(\mathbf{u} \cdot \mathbf{a}) + \mathbf{B}_Z + \mathbf{B}_{\text{demag}}, \quad (2.13)$$

and so, the torque acting on the magnetic moments vanishes $\mathbf{M} \times \mathbf{B}_{\text{eff}} = 0$.

2.1.5 The Landau-Lifshitz-Gilbert equation

Finding an equilibrium magnetisation via minimisation of equation (2.5) may not always result in physically meaningful distributions. This is because “the energy landscape of a micromagnetic system is usually very complicated and contains many local maxima, minima and saddle points” (Scholz, 2003). Therefore a more physical approach is finding a solution to the dynamical problem. The motion of a magnetic moment is mainly due to the Larmor precession around its local field. The Gilbert equation describes this precession and considers damping effects with a single damping constant α

$$\frac{d\mathbf{M}}{dt} = -\gamma \mathbf{M} \times \mathbf{H} + \frac{\alpha}{M_s} \mathbf{M} \times \frac{d\mathbf{M}}{dt}, \quad (2.14)$$

where $\gamma = 2.210173 \times 10^5 \frac{\text{m}}{\text{A}\cdot\text{s}}$ is the gyromagnetic ratio. This formulation is equivalent to the LLGE when damping is small

$$\frac{d\mathbf{M}}{dt} = -\gamma' \mathbf{M} \times \mathbf{H} - \frac{\alpha\gamma'}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}), \quad (2.15)$$

with $\gamma' = \frac{\gamma}{1+\alpha^2}$.

2.1.6 Micromagnetic modelling

While the fundamentals of micromagnetic theory were laid out by Landau and Lifshitz (1935) and W. F. Brown (1940) already by the first half of the 20th century, analytical treatment of the micromagnetic equations has been limited to the simpler cases like plane domain walls or

the law of approach to magnetic saturation. In order to investigate more complex situations it is necessary to turn to approximate methods. Numerical simulations of the micromagnetic equations are, in the most general case, numerically very expensive, specially the calculation of the long-range nonlinear demagnetising energy due to magnetostatic dipolar interactions. This constrained the primitive numerical investigations to one- or two-dimensional rotations of the dipoles as well as geometries. Although useful to probe the stability of ferromagnetic crystals, these constrained simulations are very limited as there is no doubt that the true nature of spin structures in ferromagnetic crystals is three-dimensional.

Williams and Dunlop (1989) conducted unconstrained three-dimensional simulations of single magnetite cubic grains, confirming the critical size of single domain magnetite grains using a conjugate gradient method for minimising the energy. Their method consisted in subdividing a cubic “sample” of magnetite into further cubes within the exchange length of the material. Inside each of the cubic cells the magnetisation is the average over a very large number of atomic spins and is represented by a magnetic dipole \mathbf{m}_i at the center of the cube. The magnitude of all the dipoles is constant but their directions are allowed to vary. Already in a sample divided into $12 \times 12 \times 12$ cells, a direct calculation of the demagnetising energy would take around 1.5 million interaction calculations per iteration. Rewriting the demagnetising energy in the manner of Rhodes and Rowlands (1954) they were able to reduce the computation significantly and solve for up to $22 \times 22 \times 22$ subcubes.

While the exchange, anisotropy and Zeeman energy are local and easily calculated, it is the nonlocal dipolar magnetostatic interactions that are the principal obstacle in scaling up simulations. Much of the effort in micromagnetic research has been directed towards creating ever more efficient ways to calculate the demagnetising energy. Fabian et al. (1996) and Wright et al. (1997) have developed and applied finite difference methods based on a fast Fourier transform to calculate the demagnetising energy. This, together with growing computing capabilities have allowed micromagnetics to move towards bigger models. Nevertheless, finite difference methods restrict the models’ geometries to cuboid (rectangular prisms more generally) shapes that, while useful, are somewhat unrealistic shapes for most magnetic minerals.

Finite element methods (FEM) have the advantage of being more flexible in regards to the geometries that can be modelled; in fact, they allow for arbitrary shapes. This advantage comes at the cost of higher mathematical complexity. However, the geometric flexibility of FEM allowed Williams et al. (2010) to model mineral grains with complex morphologies.

The minimisation of the magnetic Gibbs free energy, though useful, can lead to unphysical situations where the final configuration lies in a shallow energy minimum. Also, it is only useful to find equilibrium states and so the path taken cannot be interpreted as a physical solution that reflects the dynamics. The solution to this problem is to solve the dynamics of the system via the LLGE. Suess et al. (2002) developed a preconditioned integration method for the LLGE using a FEM. This allowed to simulate the dynamics and configurations of granular media.

The capabilities of today's computers allows to simulate not only single grains but clusters of them that interact magnetostatically with each other. This once untractable problem has been proved to be crucial and influence the critical sizes of single domain grains. Muxworthy et al. (2003) used a finite difference method and investigated the effect of magnetostatic interactions between magnetite grains on the hysteresis parameters. Muxworthy et al. (2013) used the recently measured (Chang et al., 2008) magnetic parameters of highly pure greigite to investigate the intergrain influence in chains of greigite and its implications for magnetosome crystals. These investigations can be furthered by FEM by modelling more realistic geometries and even multiple magnetic phases.

Chapter 3

Results

Chapter 4

Plan

Bibliography

- Abert, C., Exl, L., Bruckner, F., Drews, A., and Suess, D. (2013). magnum.fe: A micromagnetic finite-element simulation code based on FEniCS. *Journal of Magnetism and Magnetic Materials*, 345:29–35.
- Aldana, M., Constanzo-Alvarez, V., Vitiello, D., Colmenares, L., and Gómez, G. (1999). Framboidal magnetic minerals and their possible association to hydrocarbons: La Victoria oil field, southwestern Venezuela. *Geofís. Int.*, 38(3):137–152.
- Brown, W. F. (1963). *Micromagnetics*. Interscience, New York.
- Chang, L., Roberts, A. P., Tang, Y., Rainford, B. D., and Muxworthy, A. R. (2008). Fundamental magnetic parameters from pure synthetic greigite (Fe_3S_4). *J. Geophys. Res.*, 113(B06104).
- Costanzo-Alvarez, V., Aldana, M., Díaz, M., Bayona, G., and Ayala, C. (2006). Hydrocarbon-induced magnetic contrasts in some venezuelan and colombian oil wells. *Earth Planets Space*, 58:1401–1410.
- Díaz, M., Aldana, M., Constanzo-Alvarez, V., Silva, P., and Pérez, A. (2000). EPR and magnetic susceptibility studies in well samples from some Venezuelan oil fields. *Phys. Chem. Earth (A)*, 25(5):447–453.
- Donovan, T. J., Forgey, R. L., and Roberts, A. A. (1979). Aeromagnetic detection of diagenetic magnetite over oil fields. *Geologic Notes*, 63(2):245–248.
- Donovan, T. J., Hendricks, J. D., Roberts, A. A., and Eliason, P. T. (1984). Low-altitude aeromagnetic reconnaissance for petroleum in the Arctic National Wildlife Refuge, Alaska. *Geophysics*, 49(8):1338–1353.

- Dunlop, D. J. and Özdemir, Ö. (1997). *Rock Magnetism*. Cambridge University Press, Cambridge.
- Elmore, R. D., Imbus, S. W., Engel, M. H., and Fruit, D. (1993). Hydrocarbons and magnetizations in magnetite. In A'issaoui, D. M., McNeill, D. F., and Hurley, N. F., editors, *Applications of Paleomagnetism to Sedimentary Geology*, number 49 in SEPM Special Publication, pages 181–191, Tulsa, Oklahoma, U.S.A. SEPM (Society for Sedimentary Geology), SEPM (Society for Sedimentary Geology).
- Emmerton, S., Muxworthy, A. R., Sephton, M. A., Aldana, M., Costanzo-Alvarez, V., Bayona, G., and Williams, W. (2013). Correlating biodegradation to magnetization in oil bearing sedimentary rocks. *Geochimica et Geocosmochimica Acta*, 112:146–165.
- Fabian, K., Kirchner, A., Williams, W., Heider, F., Leibl, T., and Huber, A. (1996). Three-dimensional micromagnetic calculations for magnetite using FFT. *Geophys. J. Int.*, 124:89–104.
- Feynman, R. P., Leighton, R. B., and Sands, M. L. (1964). *The Feynman lectures on physics*. Addison-Wesley, Reading, Mass.
- González, F., Aldana, M., Constanzo-Álvarez, V., Díaz, M., and Romero, I. (2002). An integrated rock magnetic and EPR study in soil samples from a hydrocarbon prospective area. *Phys. Chem. Earth*, 27:1311–1317.
- Guzmán, O., Costanzo-Álvarez, V., Aldana, M., and Díaz, M. (2011). Study of magnetic constrasts applied to hydrocarbon exploration in the Maturín sub-basin (eastern Venezuela). *Stud. Geophys. Geod.*, 55:359–376.
- Imhoff, J. F., Meunler, G., Brunotte, X., and Sabonnadière, J. C. (1990). An original solution for unbounded electromagnetic 2D- and 3D-problemas throughout the finite element method. *IEEE Transactions on Magnetism*, 26(5):1659–1661.
- Landau, L. and Lifshitz, E. (1935). On the theory of the dispersion of magnetic permeability in ferromagnetic bodies. *Phys. Z. Sowjetunion*, 8(53).

- Liu, Q., Chan, L., Liu, Q., Li, H., Wang, F., Zhang, S., Xia, X., and Cheng, T. (2004). A study of relationship between magnetic, geochemical and mineralogical anomalies and hydrocarbon microseepage above oil and gas fields, Ordos Basin in China. *AAPG Bull.*, 88(2):241–251.
- Liu, Q., Liu, Q., Chan, L., Yang, T., Xia, X., and Cheng, T. (2006). Magnetic enhancement caused by hydrocarbon migration in the Mawangmiao oil field, Jiangnan basin, China. *Journal of Petroleum Science and Engineering*, 53:25–33.
- Liu, Q. and Liu, S. (1999). Magnetic and mineralogical characteristics of reservoir rocks in the Yakela oil field, northern Tarim Basin and their implications for magnetic detection of oil and gas accumulations. *Chin. Sci. Bull.*, 4(2):174–177.
- Machel, H. G. and Burton, E. A. (1991). Chemical and microbial processes causing anomalous magnetization in environments affected by hydrocarbon seepage. *Geophysics*, 56(5):598–605.
- Muxworthy, A., Williams, W., and Virdee, D. (2003). Effect of magnetostatic interactions on the hysteresis parameters of single-domain and pseudo-single-domain grains. *J. Geophys. Res.*, 108(B11):2517.
- Muxworthy, A. R., Williams, W., Roberts, A. P., Winklhofer, M., Chang, L., and Pósfai, M. (2013). Critical single domain grain sizes in chains of interacting greigite particles: Implications for magnetosome crystals. *Geochem. Geophys. Geosyst.*, 14(2):5430–5441.
- Reynolds, R. L., Goldhaber, M. B., and Tuttle, M. L. (1993). Sulfidization and magnetization above hydrocarbon reservoirs. In A’issoui, D. M., McNeill, D. F., and Hurley, N. F., editors, *Applications of Paleomagnetism to Sedimentary Geology*, number 49 in SEPM Special Publication, pages 167–179, Tulsa, Oklahoma, U.S.A. SEPM (Society for Sedimentary Geology), SEPM (Society for Sedimentary Geology).
- Rhodes, P. and Rowlands, G. (1954). Demagnetising energies of uniformly magnetised rectangular blocks. *Proc. Leeds Phil. Lit. Soc., Sci. Sect.*, 6:191–210.
- Scholz, W. (2003). *Scalable parallel micromagnetic solvers for magnetic nanostructures*. PhD thesis, Technischen Universität Wien.

- Suess, D., Tsiantos, V., Schrefl, T., Fidler, J., Scholz, W., Forster, H., Dittrich, R., and Miles, J. J. (2002). Time resolved micromagnetics using a preconditioned time integration method. *Journal of magnetism and magnetic materials*, 248:298–311.
- W. F. Brown, J. (1940). Theory of the approach to magnetic saturation. *Phys. Rev.*, 58(736):736–743.
- Williams, W. and Dunlop, D. J. (1989). Three-dimensional micromagnetic modelling of ferromagnetic domain structure. *Nature*, 337:634–637.
- Williams, W., Evans, M. E., and Krása, D. (2010). Micromagnetics of paleomagnetically significant mineral grains with complex morphology. *Geochem. Geophys. Geosyst.*, 11(2).
- Wright, T. M., Williams, W., and Dunlop, D. J. (1997). An improved algorithm for micromagnetics. *J. Geophys. Res.*, 102(B6):12085–12094.