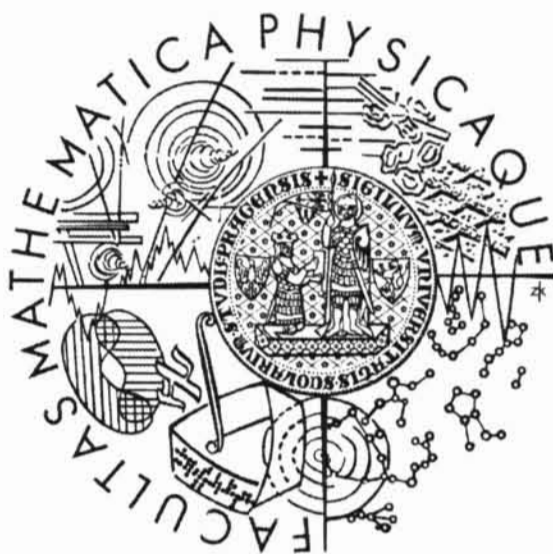


Charles University in Prague
Faculty of Mathematics and Physics

BACHELOR'S THESIS



Lukáš Vermach

Mathematical modeling of magnetostrictive materials

Mathematical Institute of Charles University

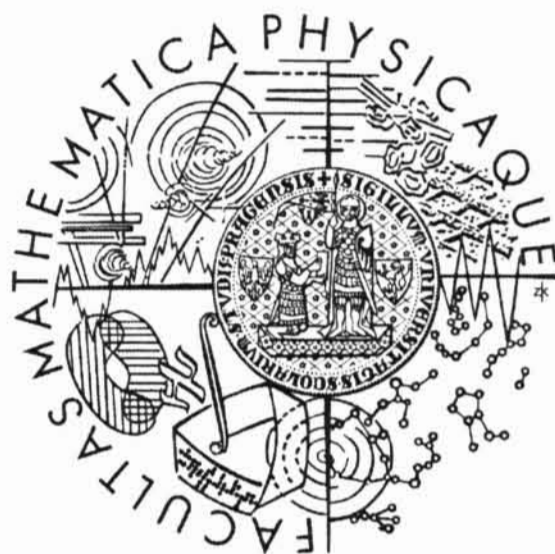
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BAKALÁŘSKÁ PRÁCE



Lukáš Vermach

Matematické modelování magnetostriktních látek

Matematický ústav Univerzity Karlovy

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Prohlašuji, že jsem svou bakalářskou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

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Lukáš Vermach



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Název práce: Matematické modelování magnetostrikčních látek
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Abstrakt

V předložené práci jsou studovány matematické aspekty modelování magnetostrikčních látek, tj. materiálu, u nichž lze měnit tvar vzorku aplikací magnetického pole nebo naopak magnetizaci namáháním vzorku. Typickým příkladem takových látek jsou magnetické slitiny s tvarovou pamětí. V práci jsou vyloženy relevantní partie matematické a fyzikální teorie mikromagnetismu a magnetostrikčních látek, je představen matematický model materiálu s magnetickou tvarovou pamětí v podobě energetického funkcionálu a následně je provedena jeho matematická analýza. Model je dále doplněn jednoduchou numerickou simulací.

Klíčová slova: Magnetická tvarová paměť; magnetostrikční látky

Title: Mathematical modeling of magnetostrictive materials
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Abstract

In the present work we study mathematical aspects of modeling of magnetostrictive materials, i.e. materials which change their shape on account of the external magnetic field or which embody magnetization in consequence of deformation. A typical example of such materials are ferromagnetic shape memory alloys. The work introduces relevant parts of mathematical and physical theory of micromagnetism and magnetostriction, and we present at the formulation of a mathematical model of a ferromagnetic shape memory alloy in the form of energy functional. Afterwards, we deal with mathematical analysis of the model and we also provide a simple numerical simulation.

Keywords: Magnetic shape memory; Magnetostrictive materials

Chapter 1

Introduction to shape memory alloys

Shape memory alloys (SMAs) are materials which are able to return to their original shape after having been deformed by applying heat to the alloy. Commonly used SMAs are typically made of copper-zinc-nickel (CuZnNi), copper-aluminium-nickel (CuAlNi) or nickel-titanium (NiTi). This unusual property of shape memory offers wide a range of applications, especially in aeronautics, piping and medicine (vascular stents).

The reason for such behavior is connected with the existence of two stable solid phases in SMAs: the high-temperature cubic phase called austenite and the low-temperature phase called martensite. The change between these two phases in SMAs is evoked by changing temperature. Moreover, there are two forms of martensite: deformed and un-deformed (twinned). The process is described by four values of temperature: A_s , A_f , M_s , M_f which determine the start and end of each phase.

While cooling in the absence of an applied load, the alloy transforms from austenite into twinned (self-accommodated) martensite. As a result of this phase transformation, no observable macroscopic shape change occurs, but at this state, the material can be easily deformed. Applying external loading to the sample leads to martensite phase transformation and the specimen moves into a deformed phase. The original shape of the body may then be reached by heating upon temperature A_f . The heat transmitted to the specimen is the energy driving the atomic rearrangement of the alloy, similar to heat that melts ice into water, but the SMAs stay solid. The deformed martensite is now transformed to the cubic austenite phase, which is configured in the original shape of the specimen. The situation is schematically shown in Figure 1.1.

Magnetostrictive materials, in general, are materials with the ability to change their shape due to an external magnetic field or embody non-vanishing magnetization associated with deformation. Ferromagnetic¹ Shape Memory Alloy Materials (FSMAs) are similar to

¹Terminological remark: Paramagnetic materials are those whose magnetic moments are randomly oriented. When an external magnetic field is applied, these moments start to align along the field. The overall magnetization is proportional to the intensity of the magnetic field. The magnetic moments of ferromagnetic materials tend to be aligned parallel to each other when an external magnetic field is applied. However, in contrast to paramagnetic materials, these moments remain parallel even when the magnetic field is removed. Another type of magnetic materials, such as ferrimagnetic or antiferromagnetic, may be

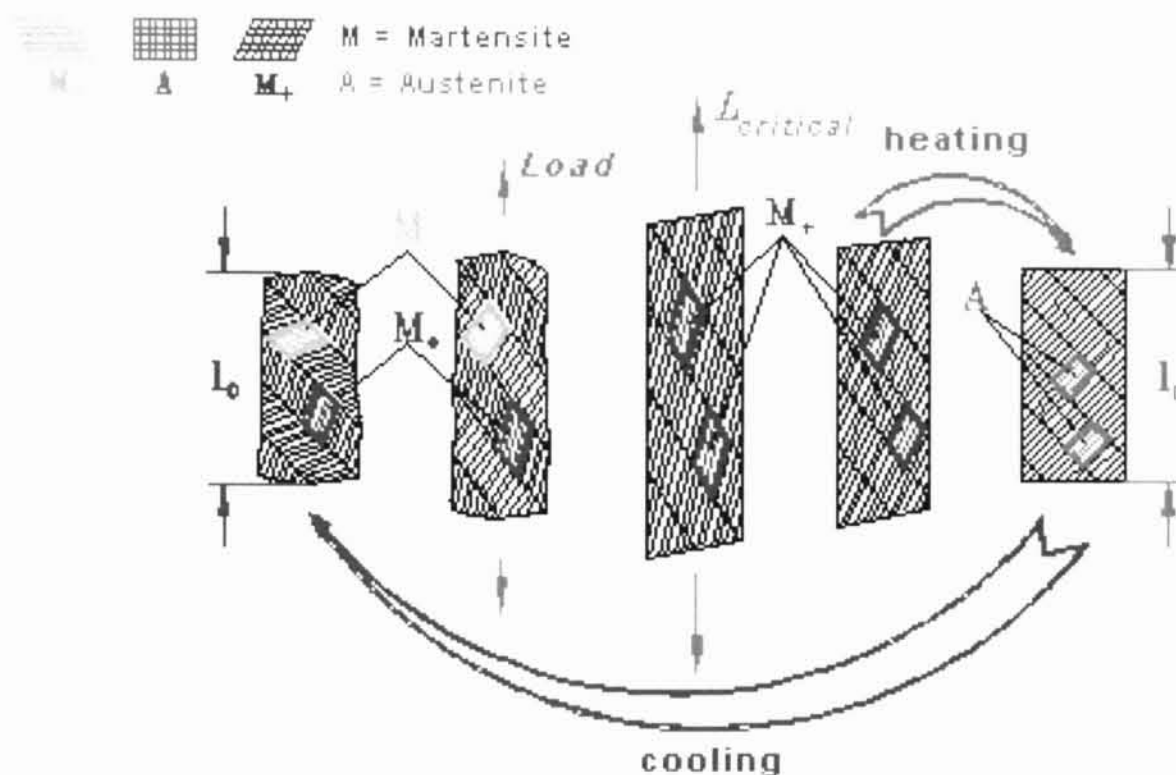


Figure 1.1: Microscopic Diagram of the Shape Memory Effect (picture overtaken from web site of Technical University Berlin <http://www.smaterial.com/SMA/sma.html>)

SMA. They embody twinning mechanism, as observed in SMA materials, however the difference is in causation of phase change. In FSMA, the phase transformation is initiated by applying an external magnetic field. For better illustration of the twinning mechanism see Figure 1.2.

The effect of magnetostriction could be understood through the domain structure of a ferromagnetic body and energy associated with this structure. Domains are regions of approximately constant magnetization. In the demagnetized state the specimen adopts magnetic domain alignment with zero net magnetization in order to bring down the magnetostatic energy. Most common type of magnetostriction is so called Joule magnetostriction, where the dimension change is connected with a redistribution of domain structures responding to an applied external magnetic field. Each of the magnetic domains is distorted by interatomic forces in a way so as to minimize the total energy of the sample.

Considering one of these domains, material with positive (negative) magnetostriction embodies extension (contraction) of a domain along magnetization direction while simultaneously contraction (extension) perpendicular to magnetization direction, keeping constant volume (see the Figure 1.3). The magnetostrictive body is a complex of many magnetostrictly distorted domains. Applying the external magnetic field causes dislocation of boundaries between magnetic domains and rotation of magnetization direction within a domain to achieve the "satisfactory" location (with lowest total energy). This is accompanied with growth of domains which have magnetization direction close to the field direction, at the cost of domains which magnetization direction differs more from the field direction. These two mechanisms result in macroscopic dimension change of the specimen. The process of reorientation of domains is far more complicated. However the main idea remains, that the rotation and the movement of magnetic domains cause deformation of the shape

found in literature. For more information see [10].

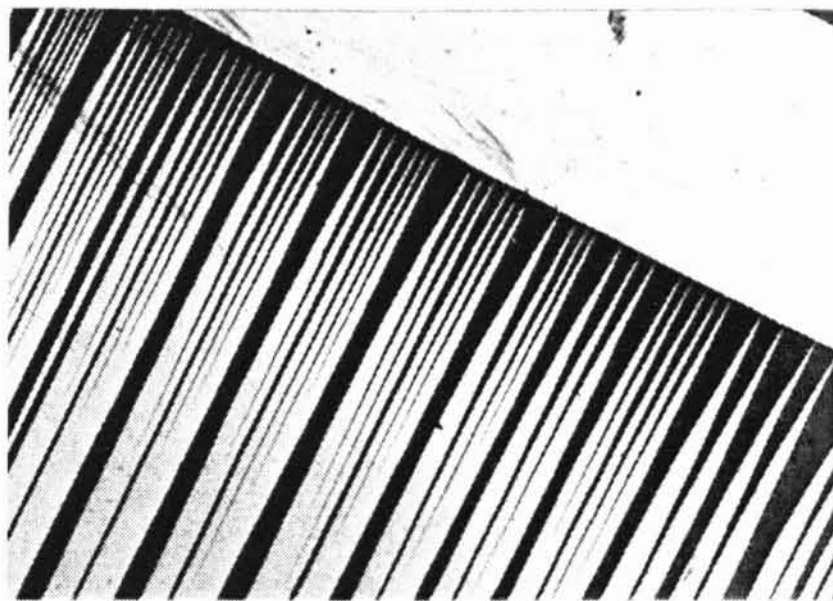


Figure 1.2: Microscopic twinning structure of CuAlNi with austenite-martensite interface. Figure used with of courtesy C. Chu, R.D. James.

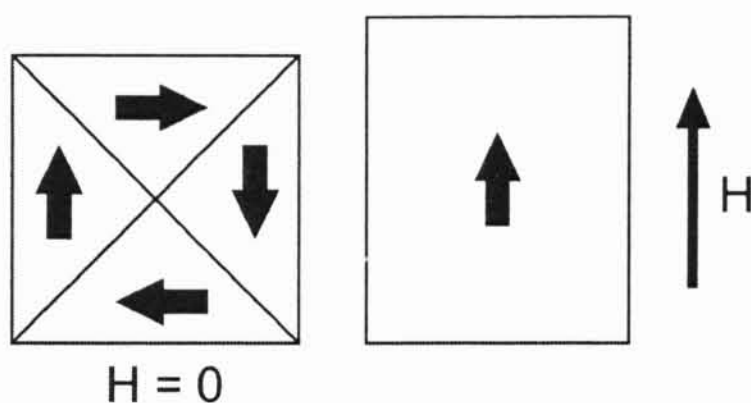


Figure 1.3: Schematic representation of a possible domain structure in a single crystal before and after applying magnetic field

of the material (for more detailed discussion, see e.g. [1] or [9]).

Magnetostrictive materials are interesting due to their application potential. FSMAs may be used for the construction of the sensors and transducing components in modern machineries. The actuation mechanism is always provided by energy transformation (electric/magnetic, thermal) into the mechanical work. The component needs to combine large strains, high-force production and fast dynamic response during an actuation event. FSMAs have potential to satisfy these requirements. Hence Reaction Mass Actuator, Wireless Linear Micro-Motor, Terfenol-D Wireless Rotational Motor, Terfenol-D Electro-Hydraulic Actuator, Magnetostrictive Contact-less Torque Sensor and many other applications were introduced in related literature. For further and a more detailed description about state-of-art applications of magnetostrictive materials see e.g. Olabi [14], Chernenko [2].

The aim of this work is to become familiar with the mathematical and physical theory of linear elasticity, micromagnetism and magnetostrictive materials, as well as to study the behavior of ferromagnetic shape memory alloys via a simple mathematical model. We start from the assumption that the material is continuous, neglecting microscopic consequences. Therefore, considering small deformation, several results of continuum mechanics are introduced in Chapter 2 to justify using the minimum total potential energy principle. In Chapter 3, the mathematical model of micromagnetism is presented and we also discuss

the application of "The Direct Method" to prove the existence of energy minimizers. Finally, a model combining linear elasticity and micromagnetism is introduced in Chapter 4. In terms of solvability, mathematical formulation of ferromagnetic shape memory model is rather complex and far from being simple. Hence a relaxed problem is formulated and discussed, and the existence of a solution is proved under certain conditions. In addition, we provide a numerical model of a wire made from magnetostrictive material. The effect of hysteresis is taken into consideration.

Chapter 2

Linear elasticity

In this chapter, we review some results derived in continuum mechanics, which are important for the description of magnetostrictive material. In Section 2.1, we focus on a mathematical representation of continuum body and its motion (kinematics). Section 2 deals with the description of motion causer (stress) and its relation to the change of state (Hooke's law). In Section 2.3, the classical formulation of the linear elasticity problem is given as well as derivation of minimum total potential energy principle. Finally in Section 2.4, the existence of minimizing problem set in Section 3 is presented. For comprehensive theory of linear elasticity see [8] or [13].

2.1 Kinematics

In continuum mechanics, we model a body as a set of mass points identified with the part of space $\Omega \subset \mathbb{R}^3$ that it occupies in certain time. Let Ω be open, bounded set. When the observed body is moving, the domain Ω is changing in time. Further more we assume that the body is homogeneous and Ω has a Lipschitz boundary.

Definition 2.1.1 *Let Ω be a domain. The boundary Γ of Ω is said to be Lipschitz if there exist numbers $\alpha > 0$ and $\beta > 0$ so that for $\forall x^0 \in \Gamma$ the frame of reference could be translated and rotated to the point x^0 such that the following is valid. If we denote*

$$K_{n-1} = \{x \in \mathbb{R}^n, |x_i| \leq \alpha \text{ for } \forall i = 1, \dots, n-1, \}$$

then there exists a Lipschitz function $a : K_{n-1} \rightarrow \mathbb{R}$, such that $a(x_1, \dots, x_{n-1}) = x_n$. And all $x = (x_1, \dots, x_{n-1}, x_n) \equiv (x', x_n)$ having $x' \in K_{n-1}$ and $a(x') < x_n < a(x') + \beta$ lay in Ω and all $x = (x', x_n)$ having $x' \in K_{n-1}$ and $a(x') - \beta < x_n < a(x')$ lay outside $\bar{\Omega}$.

Let us consider a one-to-one mapping $\chi : \Omega \rightarrow \mathbb{R}^3$ called configuration, assigning every point $\tilde{X} \in \Omega$ its position x in \mathbb{R}^3 . Then the motion is one-parameter configuration class $\chi_t : \Omega \rightarrow \mathbb{R}^3, t \in \mathbb{R}$:

$$x = \chi_t(\tilde{X}) = \chi(\tilde{X}, t),$$

where t represents time.

Choosing one configuration as a referential one and denoting points \tilde{X} with positions of X in referential configuration ($X = \chi_0(\tilde{X})$, $\Omega = \chi_0(\Omega X)$), we may get a useful description of motion (deformation) of the body

$$x = \chi(\tilde{X}, t) = \chi(\chi_0^{-1}(X), t) = \chi(X, t).$$

Then the one-to-one mapping $x = \chi(X, t)$ is called the deformation function with respect to referential configuration and it is known as the Lagrange representation.

In this text, we will be interested in changes between referential configuration Ω and current configuration Ω , but not in the way in which the change occurs. This means that time evolution is not relevant for us and we may write $x = \chi(X, t) = \chi(X)$.

In view of the description above, the local geometrical transition surrounding of an arbitrary point of the body is defined by the deformation gradient

$$F = \nabla \chi = \nabla x \quad F_{ij} = \frac{\partial \chi_i}{\partial X_j} = \frac{\partial x_i}{\partial X_j}.$$

To avoid the disappearance of the mass, we assume $\det F > 0$. Thus, the deformation of any linear element dX is given by $dx = FdX$, and for the square of the change of length of this element we obtain

$$|dx|^2 - |dX|^2 = |FdX|^2 - |dX|^2 = dX F F^T dX - dX dX = dX (F F^T - 1) dX.$$

The term $E = \frac{1}{2}(F^T F - 1)$ is called the tensor of finite deformation. It is useful in introducing field quantity $u : \Omega_0 \rightarrow \Omega$ as $u(X) = \chi(X) - X$ describing the displacement of points from referential to current configuration. Then $\nabla u = F - 1$ and the tensor of finite deformation looks as follows:

$$E = \frac{1}{2} [(\nabla u + 1)^T (\nabla u + 1) - 1] = \frac{1}{2} [\nabla u + (\nabla u)^T + (\nabla u)^T (\nabla u)]$$

If we restrict our attention to small deformations $|\nabla u| \ll 1$ and neglect the last term in the last equation, we obtain the so-called small deformation tensor

$$e = \frac{1}{2} [\nabla u + (\nabla u)^T],$$

which also gives the precise meaning of the displacement gradient. Considering the decomposition of the displacement gradient into the symmetric and antisymmetric parts, we see that each transformation could be represented by composition of a pure deformation and a pure rotation:

$$\nabla u = \underbrace{\frac{1}{2} [\nabla u + (\nabla u)^T]}_{\text{deformation}} + \underbrace{\frac{1}{2} [\nabla u - (\nabla u)^T]}_{\text{infinitesimal rotation}}.$$

2.2 Primal problem of linear elasticity formulation

The state of continuum subjected to an applied external force is well described by Cauchy's stress tensor. Forces acting within the body could be divided into body forces (e.g. gravitation) and contact forces (e.g. press, friction).

Let $\Omega^0 \subset \Omega$ with Lipschitz boundary Γ^0 , $x \in \Gamma^0$ and ν be the outer normal to Γ^0 in x . The stress vector $T(x, \nu)$, $T : \Omega \times S \rightarrow \mathbb{R}^3$, where S denotes unit sphere, characterizes the density of contact forces acting from $\Omega - \Omega^0$ to $\bar{\Omega}^0$ in point x . Then the relation between stress and outer normal is intended by Cauchy's theorem.

Theorem 2.2.1 *Let us assume $T \in C(\bar{\Omega} \times S)$. Then $T(x, \nu)$ is linearly dependent on ν in x , i.e. there exists tensor τ such as*

$$T(x, \nu) = \tau(x)\nu(x)$$

for $\forall x \in \Omega^0$ and any $\nu(x)$ in x .

We use the Einstein summation convention. Proof of the statement can be found in [13]. The following equilibrium equations shows important properties of stress tensor.

Theorem 2.2.2 *Let us assume $\tau \in C^1(\Omega)$. Let $F : \Omega \rightarrow \mathbb{R}^3$ be a body force density. Let $x^0 \in \Omega$ and $\Omega_h \subset \Omega$ be a ball with Lipschitz boundary with center in x^0 and radius h . Then*

1. (force equilibrium)

$$\frac{\partial \tau_{ij}}{\partial x_j}(x^0) + F_i(x^0) = 0, \quad \text{for } i = 1, 2, 3 \text{ and } \forall x^0 \in \Omega \quad (2.1)$$

2. (force momentum equilibrium)

$$\tau_{ij} = \tau_{ji}, \quad \text{for } \forall i, j \text{ and } \forall x^0 \in \Omega \quad (2.2)$$

Generally in mechanics, we are concerned with a position change (characterized by the deformation tensor) of the body in relation to applied external forces (described by the stress tensor). The response of one material to a loading may vary according to the measure of applied stress. Therefore we distinguish plastic deformation, where the specimen stays deformed after unloading and elastic deformation, whereas the body takes back its own shape after removing the stress. In this text, we restrict our attention to the situation when the stress depends linearly to the deformation of a specimen. This is usually called the linear theory of elasticity. The assumption set above may be expressed by Hooke's law

$$\tau_{ij}(x) = \mathbb{C}_{ijkl}(x)e_{kl}(x) \quad \text{for } i, j = 1, 2, 3. \quad (2.3)$$

for $\forall x \in \Omega$, where $\mathbb{C}_{ijkl} \in \mathbb{R}$. In this equation, no absolute term occurs since we assume, that if the deformation tensor equates to zero, then the stress vanishes as well. From symmetry of τ and e , we obtain

$$\mathbb{C}_{ijkl} = \mathbb{C}_{jikl} \quad \text{and} \quad \mathbb{C}_{ijkl} = \mathbb{C}_{ijlk}.$$

In addition to this, energy considerations give

$$\mathbb{C}_{ijkl} = \mathbb{C}_{klij}.$$

Generally, there are 21 constants describing the material. This number could be cut down for some materials, but for example copper sulphate has 21 independent constants.

Definition 2.2.3 *The material is said to be homogenous, if $\mathbb{C}_{ijkl}(x) = \mathbb{C}_{ijkl}$ for $\forall x \in \Omega$. The material is said to be isotropic in $x \in \Omega$, if $\mathbb{C}_{ijkl}(x)$ is independent of the choice of coordinates.*

For isotropic materials the Generalized Hooke's law holds:

$$\tau(x) = \lambda \text{Tr}(e(x)) + 2\mu e(x) \quad (2.4)$$

or written in components

$$\tau_{ij}(x) = \lambda e_{ij} \delta_{ij} + 2\mu e_{ij}(x), \quad (2.5)$$

where λ, μ are so-called Lamé's constants.

Remark 2.2.4 $\lambda = \mathbb{C}_{1122}$, $\mu = \mathbb{C}_{1212}$.

If we assume $u \in C^2(\Omega)$, $F \in C^1(\bar{\Omega})$ and that the equilibrium equations are satisfied in Ω , we may then formulate the linear elasticity primal problem. Substituting the equation into the force equilibrium from the Generalized Hooke's law, we obtain

$$\frac{\partial}{\partial x_i}(\lambda e_{ii}) + \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_i}{\partial x_j} \right) + \frac{\partial}{\partial x_i} \left(\mu \frac{\partial u_j}{\partial x_i} \right) + F_i = 0 \quad (2.6)$$

$$(\lambda + \mu) \frac{\partial e_{ii}}{\partial x_i} + \mu \Delta u_i + F_i = 0 \quad (2.7)$$

for $i = 1, 2, 3$, where we used the homogeneity of the body. The two sets of equations are the so-called general Lamé's equations and Lamé's equations for homogenous and isotropic bodies.

Definition 2.2.5 *Let Ω be a domain with Lipschitz boundary Γ . Let Γ_1, Γ_2 be disjoint and open in Γ such that $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \tilde{\Gamma}$, where $\tilde{\Gamma}$ has zero surface measure. There are contact forces $T : \Gamma_1 \rightarrow \mathbb{R}^3$ given on Γ_1 and boundary displacement $u^0 : \Gamma_2 \rightarrow \mathbb{R}^3$ given on Γ_2 . λ, μ are Lamé's constants. Then the primal problem of the linear elasticity is to find*

$$u \in C^1(\Omega \cup \Gamma_1) \cap C(\Omega \cup \Gamma_2) \cap C^2(\Omega)$$

satisfying (2.4) and

$$\tau_{ij} \nu_j = T_i \quad \text{on } \Gamma_1, \quad (2.8)$$

$$u = u^0 \quad \text{on } \Gamma_2, \quad (2.9)$$

where $T \in C(\Gamma_1)$ and $u^0 \in C(\Gamma_2)$.

The boundary condition (2.4) can be expressed using generalized Hooke's law

$$\lambda e_{ii} \nu_i + 2\mu e_{ij} \nu_j = T_i \quad \text{on } \Gamma_1. \quad (2.10)$$

2.3 The minimum potential energy principle

The equilibrium equations presented in Theorem (2.2.2) enable us to describe the stability of any part of the body. These differential equations holds for every point of the specimen and have a local character. The equilibrium can also be described by integral relations using the energy balance or a variational principle for energy. This way of characterization turns out to be very useful for mathematical analysis and approximative solutions.

Let us consider $\tau(x)$ and $u(x)$ satisfying conditions (2.8), (2.9) and the force equilibrium equation. We assume, that $\tau(x)$ and $u(x)$ are smooth enough so that the Green's Theorem is valid and all differential relations and boundary conditions make sense.

If we then rewrite (2.1) in integral formulation and apply Green's Theorem, we obtain

$$\int_{\Omega} \tau \cdot e(u) \, dx = \int_{\Omega} F u \, dx + \int_{\Gamma_1} T u \, dS + \int_{\Gamma_2} \nu^T \tau u^0 \, dS. \quad (2.11)$$

The equation above can be interpreted in such a way, that (virtual) work of inner forces equates to the (virtual) work of outer (body and contact) forces. This is the so-called virtual work principle.

Furthermore, we may consider τ_0 and fields of displacement u_0 , $u_0 + \delta u$ all complying with the primal problem of linear elasticity. If we put these into (2.11) and deduct the equations from each other, we get

$$\int_{\Omega} \tau_0 \cdot e(\delta u) \, dx = \int_{\Omega} F \delta u \, dx + \int_{\Gamma_1} T \delta u \, dS. \quad (2.12)$$

We reflect $\delta e(u) = e(\delta u)$, where δu stands for variation of u (virtual displacement). Relation (2.12) expresses the virtual displacement principle.

For deriving the minimum potential energy principle, it is enough to use Hooke's law for anisotropic material (2.3) and substitute it into the virtual displacement principle. We presume that \mathbb{C} is positive definite, which is to say, there exist $c_0 > 0$ such that

$$\langle \mathbb{C}e(u), e(u) \rangle \geq c_0 e(u) \cdot e(u),$$

$\forall e : e = e^T$. Let τ_0 , u_0 satisfy the primal problem of linear elasticity. Since

$$\frac{1}{2} \delta \langle \mathbb{C}e(u_0), e(u_0) \rangle = \frac{1}{2} \frac{d}{dt} \langle \mathbb{C}e(u_0 + t\delta), e(u_0 + t\delta u) \rangle |_{t=0} = \langle \mathbb{C}e(u_0), e(\delta u) \rangle,$$

where \langle, \rangle stands for the dot product, we obtain

$$\frac{1}{2} \int_{\Omega} \langle \mathbb{C}e(u_0), \delta e(u) \rangle \, dx - \int_{\Omega} F \delta u \, dx - \int_{\Gamma_1} T \delta u \, dS = 0,$$

which can be rewritten as

$$\delta \left\{ \frac{1}{2} \int_{\Omega} \langle \mathbb{C}e(u), e(u) \rangle \, dx - \int_{\Omega} F u \, dx - \int_{\Gamma_1} T u \, dS \right\}_{u=u_0} = 0. \quad (2.13)$$

Let us denote the term in the vinculum $I(u)$ and call it the potential energy of an elastic body. It is obvious that for $u = u_0$, the functional $I(u)$ satisfies Euler's necessary condition for being the extremizer. For proof that $I(u_0)$ is minimizer see [13].

The minimum potential energy minimizer could be then formulated. If u_0 is the solution of the linear elasticity primal problem then u^0 gives

$$I(u) = \frac{1}{2} \int_{\Omega} \langle \mathbb{C}e(u), e(u) \rangle dx - \int_{\Omega} Fu dx - \int_{\Gamma_1} Tu dS,$$

the lowest value amongst u complying with (2.8), (2.9). At this point, the question of existence of such a minimizer arises. We will return to this matter later in Chapter 3.

Chapter 3

Micromagnetism

In the previous chapter, we built a formalism in order to describe the behavior of a continuous body subjected to a external body and contact forces, and we justified the potential energy approach to the problem. In this chapter, we develop our concept considering magnetically active body. We formulate the term for the potential energy of such a material in Section 3.1. Moreover, in Section 3.2, we introduce the direct proof of existence of the energy minimizer and finally in Section 3.3, we do the same for the linear elasticity problem.

3.1 The potential energy of a ferromagnetic body

We study behavior of a ferromagnetic body placed in an external magnetic field H . We assume a rigid, homogeneous body identified with the part of space $\Omega \subset \mathbb{R}^3$ that it occupies. Let Ω be an open, bounded set with a Lipschitz boundary. The state of a ferromagnetic body at a fixed temperature below the Curie point is described by vector field called the magnetization $m: \Omega \rightarrow \mathbb{R}^3$, which corresponds to volume density of the macroscopic magnetic moment. This means that m generates a magnetic field u at all points of space. We assume that a ferromagnetic body could be locally saturated, i.e. there exists a value m_s , so that

$$0 < |m(\mathbf{x})| = m_s \quad \text{almost everywhere in } \Omega, \quad (3.1)$$

so that a specimen can reach a demagnetized state only in the sense of mean value. The value m_s is called saturation magnetization and in general, is a function of temperature. For the purposes of this text put $m_s = 1$. We suppose that $m(x) \in L^2(\Omega, \mathbb{R}^3)$.

The total potential energy of a ferromagnetic body exposed to an external magnetic field is composed from several contributions originating from the microscopic structure of the specimen and the properties of applied outer field. The respective components are called exchange energy, anisotropy energy, interaction energy and magnetostatic energy.

The principle of magnetism is the existence of current loops of electrons "orbiting" about a nucleus and the existence of electron spin. The exchange interaction is a quantum mechanical effect contributing to the total potential energy of the body with a spin-spin

interaction between every pair of particles having non-zero spin. There is no classical analogy for such an effect in classical mechanics. The exchange interaction contributes to the Hamiltonian of the system by term

$$H_{ex} = -\frac{1}{2} \sum J_{ij} S_i \cdot S_j.$$

where J_{ij} is the exchange integral and S_i, S_j stand for the spin operators. The summation goes through every couple (i, j) of particles taking part in the spin-spin interaction. Computation of J is based on wave function properties of the concerned particles. For more detailed information see [9]. Hence J_{ij} decreases rapidly with an increasing distance of particles we may write J instead of J_{ij} . If we substitute the spin operators with vectors and rewrite the dot product, we obtain the term for the exchange energy

$$E_{ex} = JS^2 \sum \cos \varphi_{ij}$$

where φ denotes the angle between the concerned vectors. Since only small values of φ are supposed, the Taylor's series for the cosine can be used. After shifting the zero value of energy (in order to remove any absolute term), we obtain

$$E_{ex} = JS^2 \sum \varphi_{ij}^2.$$

Notice that we take each interacting pair only once. If considered

$$|\varphi_{ij}| \approx |m_i - m_j| \approx |(r_{ij} \cdot \nabla)m|,$$

where r_{ij} stands for position vector from the lattice point i to j , then

$$E_{ex} = JS^2 \sum_i \sum_{r_{ij}} |(r_{ij} \cdot \nabla)m|^2.$$

Passing from the first summation to integration over the ferromagnetic body, the term for the exchange energy is given by

$$E_{ex} = \epsilon \int_{\Omega} |\nabla m(x)|^2 dx, \quad (3.2)$$

where $\epsilon > 0$. The exchange energy represents the ability for a specimen to create domain structure (regions of uniform magnetization), by penalizing spatial changes of m . To see this, consider the Pauli Exclusion Principle. Two electrons having different spin can stay at the same orbital, which means to have the same angular state. But the closer electrons are to each other, the stronger Coulomb repulsion they experience. On the other hand, if two electrons have the same spin, they occupy different orbits and so their relative Coulombic repulsion is lower. The Coulombic repulsion force the electron spins to be placed in different orbits, it is to say to be parallel within as large region as other effects enable.

If there was only an exchange part of the energy, the sample would adopt the single domain structure and would behave as a block magnet, which exhibits an external magnetic field with certain energy. This energy can be minimized by decreasing the external magnetic field by dividing the material into domains, see Figure 3.1. Adding extra domains increases the exchange energy because the domains can have parallel magnetization. However the total energy is decreased as the magnetostatic energy is the dominant effect. The contribution of the energy of the generated magnetic field to the total energy can be reduced to zero by a closed domain structure which does not leave any external field.

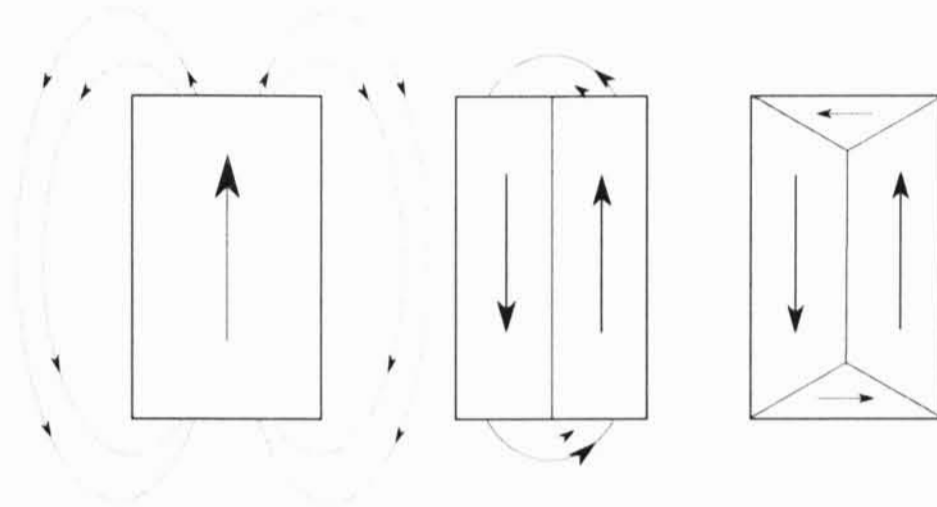


Figure 3.1: Adopting the domain structure in order to minimize the magnetostatic energy of the specimen.

In order to describe this effect, the magnetostatic energy corresponding to the energy of the magnetic field $h \in L^2(\mathbb{R}^3, \mathbb{R}^3)$ generated by magnetized body with magnetization m , need to be introduced. The induced field has to be a solution of Maxwell's equations of magnetostatics (no free currents and no electric field is concerned).

$$\begin{aligned} \operatorname{curl} h &= 0 \\ \operatorname{div}(\mu_0 h + m\chi_\Omega) &= 0 \end{aligned}$$

in \mathbb{R}^3 , where $\chi_\Omega : \mathbb{R}^n \rightarrow \{0, 1\}$ is the characteristic function of Ω and μ_0 is the vacuum permeability. Hence h is a curl-free field, and there exists a scalar function $u_m : \mathbb{R} \rightarrow \mathbb{R}^3$ called scalar magnetic potential of spatially located magnetic dipoles so that

$$h = -\nabla u_m.$$

u_m is then governed by

$$\operatorname{div}(-\mu_0 \nabla u_m + m\chi_\Omega) = 0. \quad (3.3)$$

The magnetostatic energy is the main reason for arising the domain structure.

But crystalline solids are rather anisotropic. This has the energy functional to reflect, otherwise the magnetization would always vanish if no magnetic field is applied, which does not corresponds to the observation. In magnetic crystal, there exist preferred directions, so-called easy axis, along which the physical properties could vary dramatically from others. This effect is modeled through an even, non-negative anisotropy density $\phi : B_1 \rightarrow [0, +\infty)$.

$\phi(x)$ vanishes along easy axis and thereby the directions of easy magnetization are determinate. The anisotropy energy is then given by

$$E_{ani} = \int_{\Omega} \phi(m) dx. \quad (3.4)$$

The anisotropy energy can be minimized by adopting domain structure with magnetization point along the easy axis. The ideal magnetic material has an easy axis perpendicular to one another in order to minimize both the magnetostatic and anisotropic energy (see figure 3.1 (left)). In the regions bordering the domains, so-called domain walls, there is a change in the direction of the magnetization and so magnetization is not aligned along easy axes. Hence, structure with large domains with few domain walls tend to decrease the anisotropy energy.

The interaction energy is work needed for magnetization of a specimen by a certain external magnetic field $H : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ in certain direction

$$E_{int} = - \int_{\Omega} H \cdot m dx, \quad (3.5)$$

where we assume $H \in L^1$.

The total potential energy of the ferromagnetic body, the so-called Helmholtz energy, subjected to an external magnetic field is then given by

$$I_m(m) = \epsilon \int_{\Omega} |\nabla m|^2 + \int_{\Omega} \phi(m) - \int_{\Omega} H \cdot m + \frac{\mu_0}{2} \int_{\mathbb{R}^3} |\nabla u_m|^2, \quad (3.6)$$

and in accordance with the spirit of Hamilton's variation principle, the state of the ferromagnetic body corresponds to the minimizer of the Helmholtz energy functional. The constant scaling the magnetostatic energy is vacuum permeability ¹.

Our task is to find $m_0 \in \mathcal{M}$, where $\mathcal{M} = \{m \in W^{1,2}(\Omega, \mathbb{R}^3) : |m(x)| = 1 \text{ a.e.}\}^2$, so that

$$I(m_0) = \inf \{I(m) : m \in \mathcal{M}\}.$$

3.2 The existence of the potential energy minimizer

Before we approach to prove the existence of the minimizer, it is necessary to define a few terms and give several statements, which we use hereinafter. For more a detailed introduction to the issue, see [13].

Definition 3.2.1 *Let X be a Banach space and let $f : X \rightarrow \mathbb{R} \cup \{\infty\}$*

¹The value of vacuum permeability is $\mu_0 = 4\pi \cdot 10^{-7} \text{NA}^{-2}$

² $W^{1,2}$ stands for Sobolev Space

1. f is said to be convex if

$$\lambda f(x) + (1 - \lambda)f(y) \geq f(\lambda x + (1 - \lambda)y).$$

for every $x, y \in X, \lambda \in [0, 1]$

2. f is said to be (sequentially) lower semicontinuous if

$$\liminf_{x_n \rightarrow \tilde{x}} f(x_n) \geq f(\tilde{x}).$$

3. f is said to be (sequentially) weakly lower semicontinuous over X if

$$\liminf_{n \rightarrow \infty} f(x_n) \geq f(x) \quad \text{whenever } x_n \rightharpoonup x \text{ in } X.$$

4. f is said to be coercive over X if

$$f(x) \geq \alpha \|x\| + \beta$$

for every $x \in X$ and for some $\alpha > 0, \beta \in \mathbb{R}$.

Lemma 3.2.2 (Korn's inequality.) Let Ω be an open, connected domain in \mathbb{R}^3 and $u \in W^{1,2}$. Then

$$\int_{\Omega} e_{ij}(u)e_{ij}(u)dx \geq \frac{1}{2} \int_{\Omega} \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} dx. \quad (3.7)$$

The Einstein summation convention is being used here.

Proof: Because $W^{1,2}(\Omega) = \overline{D(\Omega)}$ ³ we may assume, that $u \in D(\Omega)$. Hence

$$\frac{1}{4} \int_{\Omega} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \right) \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_i}{\partial x_j} \right) dx = \frac{1}{2} \int_{\Omega} \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} dx + \frac{1}{2} \int_{\Omega} \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} dx.$$

But for the second integral on the right side, we get (by using the integration by parts)

$$\frac{1}{2} \int_{\Omega} \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} dx = \frac{1}{2} \int_{\Omega} \left(\frac{\partial u_i}{\partial x_j} \right)^2 dx \geq 0.$$

Using this and the equation above, we obtain the statement.

Lemma 3.2.3 (Poincaré inequality.) Assume that $1 < p < \infty$ and that Ω is a bounded open subset of \mathbb{R}^n having Lipschitz boundary. Then there exists $C \in \mathbb{R}$ such that, for every function $u \in W^{1,p}(\Omega)$

$$\|u - u_{\Omega}\|_{L^p(\Omega)} \leq C \|\nabla u\|_{L^p(\Omega)},$$

where

$$u_{\Omega} = \frac{1}{|\Omega|} \int_{\Omega} u(y) dy$$

is the average value of u over Ω , with $|\Omega|$ standing for the Lebesgue measure of the domain Ω .

³ $D(\Omega)$ is a space of functions with compact support.

Theorem 3.2.4 *Let X be a reflexive Banach space and let $I : X \rightarrow \mathbb{R} \cup \{\infty\}$ be weakly lower semicontinuous and coercive over X . Assume also that there exists $\tilde{u} \in X$ with $I(\tilde{u}) < \infty$. Then there exists at least one $u_0 \in X$ such that*

$$I(u_0) = \inf \{I(u) : u \in X\} \quad (3.8)$$

Proof: Let u_n be a minimizing sequence for $\inf \{I(u) : u \in X\}$, i.e.

$$I(u_n) \rightarrow \inf I.$$

From hypotheses, we have that $\beta \leq \inf I(u) \leq I(\tilde{u}) < \infty$. Using the coercivity of I , we may then deduce that there exists $K > 0$, independent of n , such that

$$\|u_n\| \leq K.$$

Since X is reflexive, we can extract a weakly convergent subsequence still denoted u_n , such that

$$u_n \rightharpoonup u_0 \quad \text{in } X.$$

$I(u)$ is lower weakly semicontinuous, which means

$$\liminf_{n \rightarrow \infty} I(u_n) \geq I(u_0)$$

But because $\liminf_{n \rightarrow \infty} I(u_n) = \inf I$ then $\inf I = I(u_0)$.

Let us turn our attention back to the Helmholtz energy functional. We show that functional (3.6) takes the value of its infimum. In the first step, we prove that $\|m_k\|_{W^{1,2}} \leq C$. After that, in second step, we show that I_ϵ is weakly lower semicontinuous and that there exists $m_0 : I(m_0) = \inf \{I(m) : m \in \mathcal{M}\}$.

Step 1

The fact that $|m(x)| = 1$ implies $m \in L^\infty$ and therefore $m \in L^2$. Let m_k be a minimizing sequence:

$$I_\epsilon(m_k) = \epsilon \int_{\Omega} |\nabla m_k|^2 + \int_{\Omega} \phi(m_k) - \int_{\Omega} H \cdot m_k + \frac{\mu_0}{2} \int_{\mathbb{R}^3} |\nabla u_m|^2.$$

the function ϕ is non-negative and so $\int_{\Omega} \phi(m_k) \geq 0$. For interaction energy holds estimation $\int_{\Omega} H \cdot m_k \leq \|H\|_{L^1} \|m\|_{L^\infty}$.

For the estimation of magnetostatic energy, we apply an arbitrary testing function $v : \mathbb{R}^3 \rightarrow \mathbb{R} : \lim_{x \rightarrow \infty} v(x) = 0$ on equation (3.3)

$$\operatorname{div}(m\chi_{\Omega} - \mu_0 \nabla u_m)v = 0$$

$$\operatorname{div}(m\chi_{\Omega})v - \mu_0 \Delta u_m v = 0.$$

After integration over all of \mathbb{R}^3 and integration by parts

$$\int_{\partial\Omega} mv - \int_{\Omega} m \cdot \nabla v = \lim_{r \rightarrow \infty} \mu_0 \int_{S_r} v \nabla u_m - \mu_0 \int_{\mathbb{R}^3} \nabla u_m \cdot \nabla v,$$

where S_r stands for the sphere with radius r and is centered at the origin. According to behavior of the testing function, boundary items vanish. Specially for $v = u_m$ we obtain

$$\mu_0 \|\nabla u_m\|_{L^2}^2 = \int_{\Omega} m \cdot \nabla u_m \leq \|m\|_{L^2} \|\nabla u_m\|_{L^2}$$

$$\|\nabla u_m\|_{L^2} \leq \|m\|_{L^2}.$$

Considering $|m_k(x)| \leq 1$, we gain $0 \leq \int_{\Omega} |m_k(x)|^2 \leq |\Omega|$ and so

$$I_{\epsilon}(m_k) \geq \epsilon \|\nabla m_k\|_{L^2}^2 + C_1.$$

Furthermore, using Poincaré inequality

$$\frac{1}{\epsilon} I_{\epsilon}(m_k) + C_2 \geq \|\nabla m_k\|_{L^2}^2 \geq C_3 \|m_k\|_{L^2}^2,$$

where C_1, \dots, C_3 are constants. So we may then deduce that $I(m_k)$ is coercive and

$$\|m_k\|_{W^{1,2}} \leq C.$$

Since $\|m_k\|_{W^{1,2}}$ is bounded and $W^{1,2}$ is reflexive, we may (see Theorem A.0.5) extract a subsequence (still denoted m_k) such that

$$m_k \rightharpoonup m_0 \in W^{1,2}$$

Considering that the space $W^{1,2}$ is compact nesting in L^2 , we have

$$m_k \rightarrow m \in L^2.$$

This is equivalent to $\int_{\Omega} |m_k - m_0|^2 \rightarrow 0 \Leftrightarrow |m_0| = 1$ a.e.

Step 2

The functionals $\int_{\Omega} |\nabla m_k|^2$ and $\int_{\Omega} |\nabla u_m|^2$ are both convex and so according to Dacorogna [3] (see Theorem A.0.1), they are weakly lower semicontinuous.

Because $m_k \rightarrow m \in L^2$ and ϕ is continuous, $\phi(m_k) \rightarrow \phi(m_0)$ a.e. Furthermore, ϕ is bounded, so using Lebesgue's Theorem we obtain $\int \phi(m_k) \rightarrow \int \phi(m_0)$ a.e. The same is valid for the interaction energy by using Hölder's inequality

$$\int_{\Omega} H \cdot (m_0 - m_k) \leq \|H\|_{L^1} \|m_0 - m_k\|_{L^\infty} \rightarrow 0,$$

i.e. $\int_{\Omega} H \cdot m_k \rightarrow \int_{\Omega} H \cdot m_0$ a.e., which is stronger than the assumption of weakly lower semicontinuity required in the proof of Theorem 3.2.4.

Thus, the energy functional $I_{\epsilon}(m)$ is weakly lower semicontinuous and so, according to Theorem 3.2.4, there exists m_0 such that $I_{\epsilon}(m_0) = \inf \{I_{\epsilon}(m) : m \in \mathcal{M}\}$.

3.3 Minimizer existence for linear elasticity

The proof of the minimizer's existence of the potential energy in the linear elasticity is very similar to the previous proof. Let us recall the problem. For $\Omega \subset \mathbb{R}^3$, a bounded domain and $\Gamma_1, \Gamma_2 \subset \partial\Omega$, $u^0 \in W^{1,2}(\Gamma_2; \mathbb{R}^3)$ we denote

$$\mathcal{U} = \{u \in W^{1,2}(\Omega; \mathbb{R}^3) : \tau\nu = T \text{ on } \Gamma_1, u = u^0 \text{ on } \Gamma_2\},$$

where u stands for field of displacement, τ for the stress tensor and T represents the contact force.

We study the minimizing problem of the potential energy functional

$$I(u) = \frac{1}{2} \int_{\Omega} \langle \mathbb{C}e(u), e(u) \rangle dx - \int_{\Omega} F \cdot u dx - \int_{\Gamma_1} T \cdot u dS, \quad u \in \mathcal{U} \quad (3.9)$$

where F stands for a vector field of body force, $\mathbb{C} : \mathbb{R}^{3 \times 3} \times \mathbb{R}^{3 \times 3} \rightarrow \mathbb{R}$ is the elasticity tensor (in orthogonal coordinates represented by positively defined matrix) and $e : \mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{R}$ is the small-deformation tensor. The small deformation is connected with the displacement through

$$e = \frac{1}{2}(\nabla u + (\nabla u)^T).$$

To prove that the potential energy reaches the infimum, we will proceed similarly as before.

Let u_k be a minimizing sequence. Since \mathbb{C} is positively defined

$$I(u_k) = \frac{1}{2} \int_{\Omega} \langle \mathbb{C}e(u_k), e(u_k) \rangle dx - \int_{\Omega} F \cdot u_k dx \geq \alpha \|e(u_k)\|_{L^2}^2 - \|F\|_{L^2} \|u_k\|_{L^2}.$$

After applying Korn's and Poincaré inequalities, we obtain

$$I(u_k) + \|F\|_{L^2} \|u_k\|_{L^2} \geq \alpha \|e(u_k)\|_{L^2}^2 \geq \alpha \|\nabla u_k\|_{L^2}^2 \geq \tilde{\alpha} \|u_k\|_{L^2}^2.$$

So again we obtain the result

$$\|u_k\|_{W^{1,2}} \leq C.$$

Taking advantage of the properties of the spaces $W^{1,2}$ or L^2 (reflexivity and $W^{1,2} \hookrightarrow L^2$, see Theorem A.0.5 and Theorem A.0.6) we gain

$$u_k \rightharpoonup u \in W^{1,2}$$

$$u_k \rightarrow u \in L^2.$$

Further proceed is analogous to magnetism. Since the first part of (3.9) is convex and for the second part the Hölder's inequality is valid, the functional $I(u)$ is lower semicontinuous and coercive. And so, owing to Theorem 3.2.4, the potential energy functional reaches its infimum, i.e. there exists u_0 such that $I(u_0) = \inf \{I(u) : u \in \mathcal{U}\}$.

Chapter 4

Magneto - elasticity

In the following chapter, we will study the magnetostrictive materials, which means the combination of both effects - linear elasticity and magnetism. Generally, magnetostriction is the ability of some ferromagnetic materials to change their shape owing to an external magnetic field or to embody magnetization in consequence of deformation.

Such behavior makes us enlarge the potential energy model with the term of energy wells. This brings mathematical difficulties in to the minimizer existence argumentation because the resulting energy functional is not weakly lower semicontinuous at all. Therefore we introduce the quasiconvex formulation of the problem in section 4.1. The existence of the minimizer of a simplified magneto-elastic problem is solved in the successive section 4.2. The numerical model of a magnetostrictive wire, which is based on simplifications made in section 4.2, is computed in section 4.3.

4.1 The quasiconvex problem formulation

Potential energy of a magneto-elastic material at a fixed temperature below the Curie's temperature is, in general, given by

$$I(u, m) = \int_{\Omega} \Phi(u(x), m(x), \nabla u(x), \nabla m(x)) dx.$$

We denote

$$\mathcal{UM} = \{[u, m] \in W^{1,2}(\Omega, \mathbb{R}^6)\}$$

for $\Omega \subset \mathbb{R}^6$ a bounded domain, $\Gamma \subset \partial\Omega$. We suppose, that $\mathcal{UM} \neq \emptyset$.

As described above, we may associate the stable phase of the material with the minimum of the energy. This leads to the following problem:

$$\min \{ I(u, m); [u, m] \in \mathcal{UM} \}. \quad (4.1)$$

The difference between magneto-elasticity and the situations described in the previous two chapters lies in the assumption of existence of several local minimizers, the so-called energy

wells. Each well represents a stable phase of the specimen. The point is that the phase in which the specimen could be found may locally differ, and the laminating structure might occur.

The energy density $\Phi(u(x), m(x), \nabla u(x), \nabla m(x))$ is invariant under material symmetry transformations

$$\Phi(Qu, Qm, Q(\nabla u)Q^T, Q(\nabla m)Q^T) = \Phi(u, m, \nabla u, \nabla m) \quad \forall Q \in \text{SO}(3),$$

where $\text{SO}(3) = \{Q \in \mathbb{R}^{3 \times 3} : \det Q = 1, QQ^T = Q^T Q = I\}$. If $[e(u_0), m_0]$ corresponds to the minimizer of (4.1), then $[Qe(u_0)Q^T, Qm_0]$ corresponds to the minimizer of (4.1) as well as to each $Q \in \text{SO}(3)$. We suppose that every energy minimizer is generated from only one minimizer by means of symmetry transformations. Hence, the set of minimizers associated with $\int_{\Omega} \Phi \, dx$ has the structure

$$\mathcal{W} = \bigcup_{i=1}^N [e(u_{0i}), \pm m_{0i}],$$

and for each $i = 1, \dots, n$ there exists a symmetry transformation $Q \in \text{SO}(3)$ such that

$$[e(u_{0i}), \pm m_{0i}] = [Qe(u_{01})Q^T, Qm_{01}]. \quad (4.2)$$

Each couple $[e(u_{0i}), m_{0i}]$ is then called the energy well. Thus there are $N = 2n$ energy wells. It turns out that in real materials the positions of energy wells cannot be stationed arbitrarily. The set \mathcal{W} of the energy wells embodies symmetry properties reflecting symmetry of atomic structure of the concerned ferromagnetic material. This is usually called the pairwise compatibility of energy wells.

Definition 4.1.1 (*Pairwise compatibility conditions*) *The set $\mathcal{W} = \bigcup_{i=1}^N [e(u_{0i}), \pm m_{0i}]$ consists of N pairwise compatible magneto-elastic wells if there exist unit vectors n_{jk} , and vectors a_{jk} , $j, k = 1, \dots, N$ such that*

$$e_j - e_k = \frac{1}{2}(a_{jk} \otimes n_{jk} + n_{jk} \otimes a_{jk}) \quad (4.3)$$

$$(m_j - m_k) \cdot n_{jk} = 0, \quad (4.4)$$

for all $j, k = 1, \dots, N$.

The structure of pairwise compatible magneto-elastic wells is in fact the consequence of kinematic compatibility condition for solid-to-solid transformation and its application on magnetically active material. This was introduced by James and DeSimone in [5] and is briefly outlined in following paragraph.

It is known (see [6]) that for a diffusionless solid-to-solid phase transformation the kinematic compatibility condition between the strain tensors e_j and e_k is satisfactory if there exists a 180° rotation Q such that

$$Qe_kQ^T = e_j, \quad Q = -I + 2b \otimes b, \quad (4.5)$$

where b denotes the axis of rotation of Q . Assuming (4.5) and letting $a = 4[(e_k \cdot b \otimes b)b - e_k b]$, we obtain

$$e_j - e_k = \frac{1}{2}(a \otimes b + b \otimes a).$$

Therefore a planar interface can be formed to separate regions of the body deformed according to e_k and e_j , either with normal $n_I = b$ or with normal $n_{II} = a$. In the former case $Qn_I = n_I$ and the region is of type I, while in the latter case $Qn_{II} = n_{II}$ and the region of the body is of type II. In addition to this, let us assume, that Q is a symmetry transformation satisfying (4.2) and there exists a unique easy magnetic direction associated with each e_j , so that

$$m_j = \pm Qm_k. \quad (4.6)$$

Then the magnetic compatibility between k -th and j -th variant become a consequence of their elastic compatibility. In the case that $m_j = +Qm_k$

$$(m_j - m_k) \cdot n_I = (m_k - m_k) \cdot Qn_I = 0$$

and magneto-elastic compatibility can be achieved by taking $a_{jk} = a, n_{jk} = n_I = b$. If $m_j = -Qm_k$, then

$$(m_j - m_k) \cdot n_{II} = (m_k \cdot Qn_{II} - m_k) \cdot Qn_{II} = 0$$

and we take $a_{jk} = b, n_{jk} = n_{II} = a$.

The preceding given derivation assumes existence of rotation Q satisfying (4.5) and existence of unique magnetic direction for each e_j , so that equations (4.5) and (4.6) hold simultaneously. Despite these presumptions are not universally valid, they are sufficiently usable in most cases of practical interest.

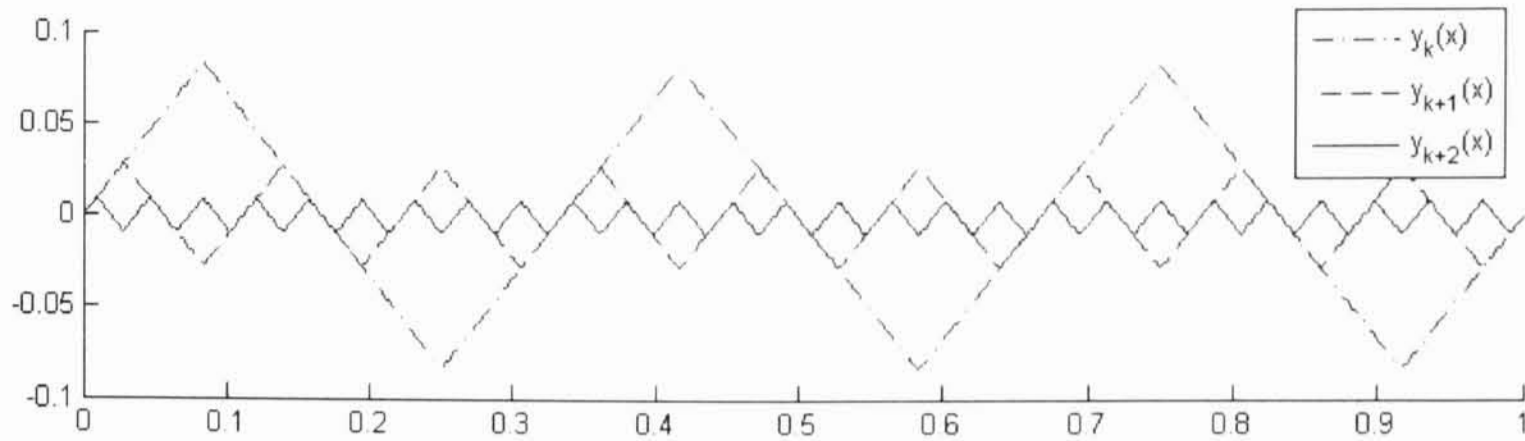
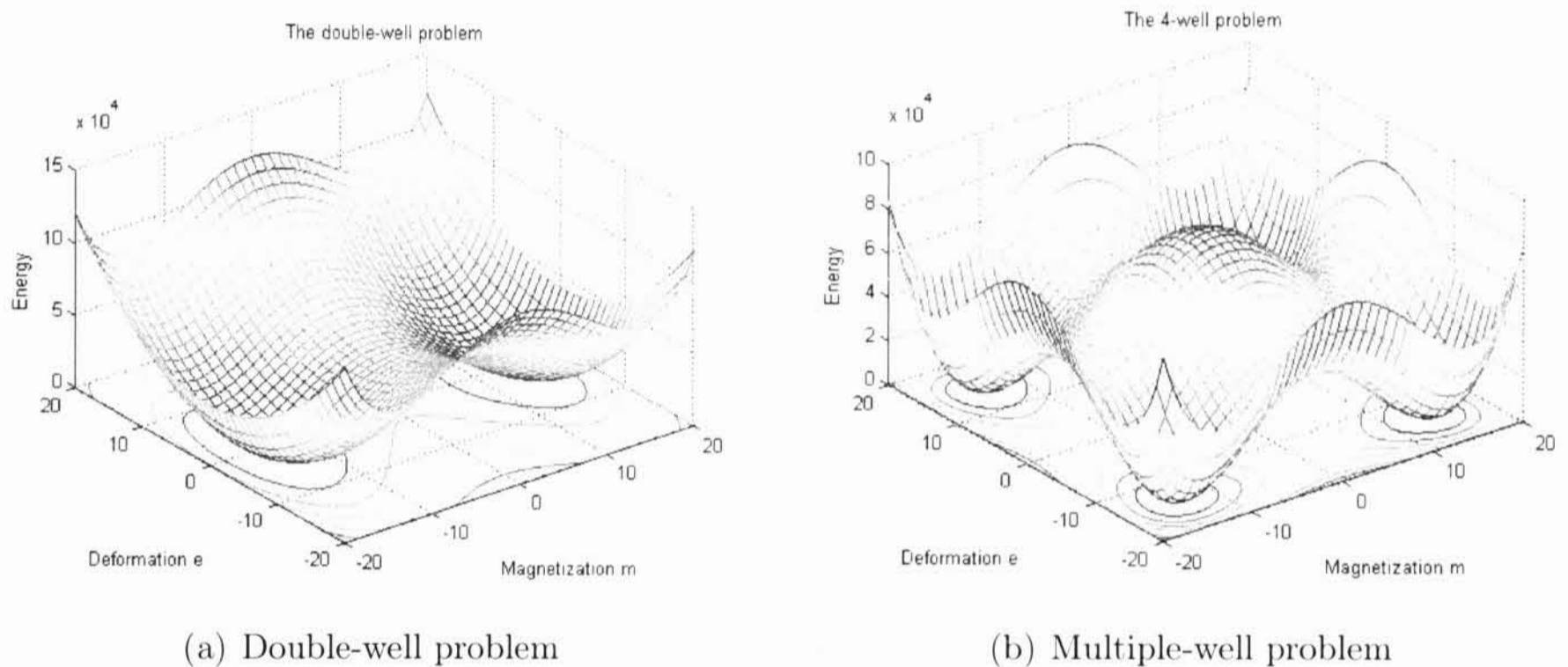
Let us turn back our attention to the minimizing problem (4.1). Generally, no solution of (4.1) exists, i.e. $I(u, m)$ does not have to reach the minimizer. To demonstrate the aforementioned situation, let us look at the following one-dimensional example.

Example 4.1.2 (*Dacorogna*)

$$\text{Minimize } J(y) = \int_0^1 y^2(x) + (y'^2(x) - 1)^2 dx, \quad y \in W^{1,4}([0, 1]), \quad y(0) = y(1) = 0.$$

It is easy to see that sequences of functions depicted on Figure 4.1 are the minimizing sequence for J and that $\lim J(y_k) = \inf J = 0$. However, $J(w - \lim y_k) = J(0) > 0$ and so the minimum is never reached. The point is that the functional J is not sequentially weak lower semicontinuous, which is the same problem we face in the model of magnetostriction. This is sometimes called double/multiple-well model (spacial oscillations among various variants of solid phase). The situation is schematically depicted on Figure 4.2.

On the other hand we saw that in linear elasticity or simply magnetism, the stable state (energy minimizer) is being reached. It is necessary to answer the question, what is the property of the energy density Φ which prevents such behavior. This condition is called quasiconvexity.


 Figure 4.1: Minimizing sequence y_k for J .


(a) Double-well problem

(b) Multiple-well problem

Figure 4.2: Schematic illustration of double-well and multiple-well problem. The energy functional of 1D specimen (e.g. wire) made from magnetostrictive material embodies two (a) four (b) local minimums.

Definition 4.1.3 $f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is said to be *quasiconvex* if for any matrix $A \in \mathbb{R}^{m \times n}$ and any smooth function $\phi : \Omega \subset \mathbb{R}^n \rightarrow \mathbb{R}^m$, $\phi(x) = Ax$, for $x \in \partial\Omega$ holds that

$$\int_{\Omega} f(\nabla\phi(x))dx \geq f(A) |\Omega|.$$

We can see that we deal with density which is not quasiconvex. Suitable extension (relaxation) of the problem, which would provide solvability, was introduced by Dacorogna (see Appendix Theorem A.0.3 or [3], Section 5.1). For the rest of this Section, let us denote the couple $[u, m] = v$, then we can reformulate the minimizing problem to

$$\min \left\{ I_Q = \int_{\Omega} Q\Phi(v(x), \nabla v(x))dx; \quad v \in \mathcal{UM} \right\}, \quad (4.7)$$

where $Q\Phi(v, \cdot)$ is the quasiconvex envelope of $\Phi(v, \cdot)$ defined by

$$Q\Phi(v, \cdot) = \sup \{ f \leq \Phi(v, \cdot); f \text{ quasiconvex} \}.$$

In such a case, I_Q is sequentially weakly lower semicontinuous and the problem (4.2) has a solution. That is to say that there is $v_0 \in \mathcal{UM}$ such that

$$I_Q(v_0) = \min \{I_Q(v) : v \in \mathcal{UM}\} \equiv \min(4.2).$$

The illustration of the idea of the quasiconvex envelope for energy functionals showed in 4.2 can be found in Figure 4.3.

The relaxed problem is connected with the original one via relaxation theorem introduced by Dacorogna, which says that under several growth conditions:

- (i) $\inf(4.1) = \min(4.2)$,
- (ii) if $v_0 \in \mathcal{UM}$ is a solution to (4.2) then there is a minimizing sequence $\{v_k\}_{k=1}^{\infty} \subset \mathcal{UM}$ converging weakly to v_0 in $W^{1,2}(\Omega, \mathbb{R}^3)$ and $\lim_{k \rightarrow \infty} I(v_k) = I_Q(v_0)$,
- (iii) any minimizing sequence of (4.1) converges weakly to the minimizer of (4.2).

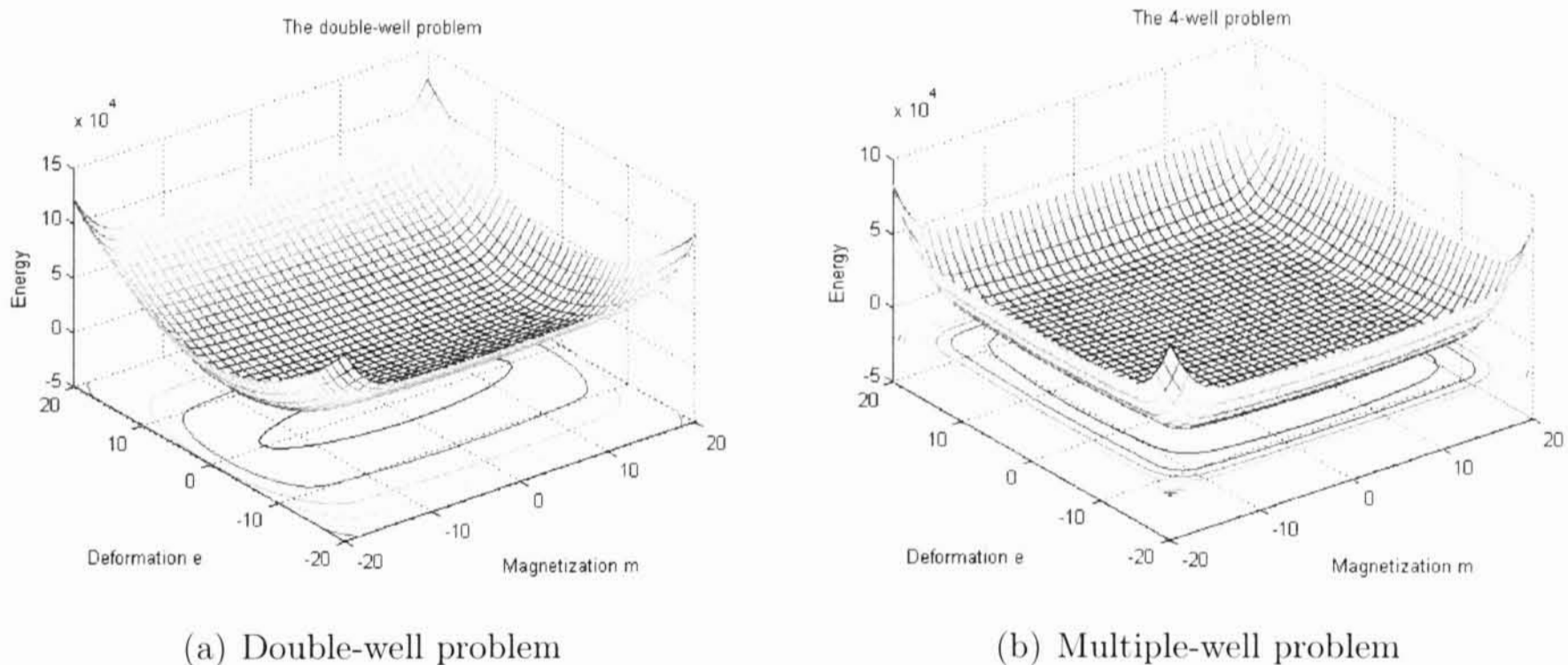


Figure 4.3: The quasiconvex envelope of the energy functional of 1D specimen made from magnetostrictive material introduced in figure 4.2.

4.2 The mathematical model of ferromagnetic shape memory alloy

Consider a magneto-elastic material having N martensitic variants. Each variant is characterized by a stress-free deformation, which is a symmetric $n \times n$ tensor ($n = 2, 3$ is the dimension), and by an easy axis prescribing two preferred directions of the magnetization $\pm m$. So, we actually face a $2N$ -well problem. As a characterizing quantity, we choose

$v : \Omega \rightarrow \mathbb{R}^{n(n+1)/2+n}$ as a conjunction of independent components of the symmetric tensor $e(u)$ and the magnetization m . For $n = 3$, we have

$$v = (e_{11}, e_{22}, e_{33}, e_{12}, e_{13}, e_{23}, m_1, m_2, m_3)$$

$$|m| = m_1^2 + m_2^2 + m_3^2 = 1$$

The i -th well is then described by the vector $v^i \in \mathbb{R}^{n(n+1)/2+n}$ where the first $n(n+1)/2$ components stay for the symmetric strain and the last n components stay for the magnetization. We assume that the set of v^i satisfies the pairwise compatibility conditions. We can group v^i , $i = 1, \dots, 2N$ so that v^{2j-1} differs from v^{2j} by the sign of the last n components $j = 1, \dots, N$.

We suppose that all variants have the same ‘‘magneto-elastic’’ moduli and that the magneto-elastic energy density of the i -th variant is given by

$$W_i(v) = \frac{1}{2} \langle \mathbb{C}(v - v^i), (v - v^i) \rangle ,$$

where $v \in \mathbb{R}^{n(n+1)/2+n}$ is the given configuration and \mathbb{C} stands for the magneto-elastic tensor. The magneto-elastic tensor is an extension of the elasticity tensor, which denotes the response of a magneto-elastic material to both deformation and external magnetic field. We presume that \mathbb{C} is positively defined. The overall energy is then

$$W(v) = \min_{1 \leq i \leq 2N} W_i(v) .$$

Notice that we know v if we know the displacement $u : \Omega \rightarrow \mathbb{R}^n$ of the body and its magnetization $m : \Omega \rightarrow \mathbb{R}^n$, $|m| = 1$ a.e. Hence, we set up the energy functional

$$I(u, m) = \int_{\Omega} W(v(x)) dx - \int_{\Omega} f \cdot u dx - \quad (4.8)$$

$$- \int_{\Gamma_1} g \cdot u dS - \int_{\Omega} H \cdot m + \frac{\mu_0}{2} \int_{\mathbb{R}^n} |\nabla u_m|^2 dx. \quad (4.9)$$

When compared with (3.6), we can see that the magnetic exchange energy was neglected. In this correction we take into consideration scaling analysis for the large body introduced by DeSimone in [4].

However, due to nonconvexity of W and because of the nonconvex constraint $|m| = 1$, the minimum of I does not necessarily exist for $u \in W^{1,2}(\Omega; \mathbb{R}^n)$, $u = u^0$ on Γ_0 and $m \in L^2(\Omega; \mathbb{R}^n)$, $|m| = 1$ because I is not sequentially weakly lower semicontinuous. Hence, we look for a weakly lower semicontinuous extension \bar{I} of I which is, generally, very difficult to find.

Following Govindjee, Mielke (see [7]) we estimate the effective energy density \bar{W} by

$$\bar{W}(\lambda, v) = \sum_{i=1}^{2N} \lambda_i W_i(v) + \frac{1}{2} \sum_{i=1}^{2N} (\lambda_i^2 - \lambda_i) \langle \mathbb{C}v^i, v^i \rangle ,$$

where $\lambda_i : \Omega \rightarrow \langle 0, 1 \rangle : 0 \leq \lambda_i, \sum_i \lambda_i = 1$ are the volume fractions of particular variants. Function $\lambda_i(x)$ expresses the relative representation of i -th phase in an infinitesimal surrounding of point x . It is easy to see that

$$\bar{W}(\lambda, v) = \frac{1}{2} \left\langle \mathbb{C} \left(v - \sum_{i=1}^{2N} \lambda_i v^i \right), \left(v - \sum_{i=1}^{2N} \lambda_i v^i \right) \right\rangle ,$$

$\lambda = (\lambda_1, \dots, \lambda_{2N})$.

Moreover, we relax the constraint $|m| = 1$ to $|m| \leq 1$.

So we define the relaxed functional

$$\bar{I}(\lambda, u, m) = \int_{\Omega} \bar{W}(\lambda(x), v(x)) dx - \int_{\Omega} f \cdot u dx - \quad (4.10)$$

$$- \int_{\Gamma_1} g \cdot u dS - \int_{\Omega} H \cdot m + \frac{\mu_0}{2} \int_{\mathbb{R}^n} |\nabla u_m|^2 dx \quad (4.11)$$

and our task is minimize it for $|m| \leq 1, m \in L^\infty(\Omega; \mathbb{R}^n), \lambda \in L^\infty(\Omega; \mathbb{R}^{2N}), u \in W^{1,2} : u = u^0$ on Γ .

To show the existence means to apply the same procedure as before. Notice that the first term of (4.10) which contains \mathbb{C} is strictly convex if \mathbb{C} is positively defined. Then for $\int_{\Omega} \bar{W}(\lambda, v) dx$ the following estimation is valid:

$$\begin{aligned} \int_{\Omega} \bar{W}(\lambda, v) dx &\geq \alpha \left\| v - \sum_{i=1}^{2N} \lambda_i v^i \right\|_{L^2}^2 \geq \\ &\geq \alpha \left| \|v\|_{L^2} - \left\| \sum_{i=1}^{2N} \lambda_i v^i \right\|_{L^2} \right|^2 \geq \alpha \|v\|_{L^2}^2 - c \|v\|_{L^2}. \end{aligned}$$

For the remaining terms of $\bar{I}(\lambda, u, m)$ we use estimations introduced in the previous chapter, i.e.

$$\begin{aligned} \int_{\Omega} H \cdot m dx + \int_{\Omega} f \cdot u dx &\leq c_m \|m\|_{L^1} + c_u \|u\|_{L^1} \leq \\ &\leq c_m \|m\|_{L^1} + \tilde{c}_u \|\nabla u\|_{L^1} \leq c \|v\|_{L^1}, \end{aligned}$$

where $c_m, c_u, \tilde{c}_u, c \in \mathbb{R}$. So finally

$$\bar{I}(\lambda, u, m) \geq \alpha \|v\|_{L^2}^2 - c \|v\|_{L^2} - c \|v\|_{L^1}.$$

Let us consider the set

$$\mathcal{H} = \{(\lambda, u, m) : |m| \leq 1, m \in L^\infty(\Omega; \mathbb{R}^n), \lambda \in L^\infty(\Omega; \mathbb{R}^{2N}), u \in W^{1,2}\}$$

and $(\lambda_k, u_k, m_k) \in \mathcal{H}$, the minimizing sequence for $\inf \bar{I}$, i.e.

$$\bar{I}(\lambda_k, u_k, m_k) \longrightarrow \inf \bar{I}.$$

We assume that $\lambda_k \rightarrow \lambda$ and $m_k \rightarrow m$. Considering estimations made above, we may deduce that $\bar{I}(\lambda_k, u_k, m_k)$ is coercive and that there exists $K \geq 0$, independent of k , such that

$$\|u_k\|_{W^{1,2}} \leq K, \quad \|m_k\|_{L^\infty} \leq K.$$

Since L^2 is reflexive Banach space and $W^{1,2} \hookrightarrow L^2$ we can extract weakly convergent subsequence (still denoted u_k) such that

$$u_k \rightharpoonup u \text{ in } W^{1,2} \quad \text{and} \quad u_k \rightarrow u \text{ in } L^2.$$

The terms $\int_{\Omega} \bar{W}(\lambda, v)$ and $\frac{\mu_0}{2} \int_{\mathbb{R}^n} |\nabla u_m|^2 dx$ are convex and so, according to Dacorogna, weakly lower semicontinuous. The remaining terms of (4.10) are continuous functionals, and u_k and m_k converge strongly. Therefore $\int_{\Omega} f \cdot u_k dx \rightarrow \int_{\Omega} f \cdot u dx$, $\int_{\Omega} H \cdot m_k dx \rightarrow \int_{\Omega} H \cdot m dx$ and $\int_{\Gamma} g \cdot u_k dS \rightarrow \int_{\Gamma} g \cdot u dS$. Hence \bar{I} is sum of weakly lower semicontinuous functionals, it is weakly lower semicontinuous as well. Considering Theorem 3.2.4, we obtain the required statement, i.e.

$$\inf \bar{I} = \bar{I}(\lambda, u, m).$$

4.3 The numerical model of a magneto-elastic wire

In this section we present a 1D example demonstrating the mathematical model described in the previous chapter. We consider a wire made from magneto-elastic material with two energy wells - two preferred directions of couple [deformation, magnetization]. We apply an external body force F , (which is in the 1D case identical to strain σ) and magnetic field H . We are interested in the response of the sample especially in stress-strain relation, magnetization-strain and stress-external magnetic field intensity dependance, as well as dependence of volume fraction on both strain and external magnetic field intensity. We assume that the energy of the specimen is given by (4.10) and (4.11), but in order to avoid numerical complication, we neglect the term with the magnetostatic potential. To justify this correction, note that the length of the wire is infinite in the view of diameter of the wire and so the contribution generated by ∇u_m vanishes. So our goal is to minimize the energy functional

$$\bar{I}(\lambda, u, m) = \int_{\Omega} \bar{W}(\lambda(x), v(x)) dx - \int_{\Omega} f \cdot u dx - \int_{\Gamma_1} g \cdot u dS - \int_{\Omega} H \cdot m \quad (4.12)$$

We model the wire as a discrete set of points x_i , $i = 0, \dots, n$, laying equidistantly along the x-axis in the interval $[0, 1]$, where $x_0 = 0$ and before loading $x_n = 1$. Quantity u_i describes the displacement of the i -th point along the x-axis. We want the sample to be

fixed on one side, therefore we set $u_0 = 0$. Let the potential energy of the specimen have the two wells at points

$$v^{01} = \begin{bmatrix} 0.05 \\ 1 \end{bmatrix} \quad \text{and} \quad v^{02} = \begin{bmatrix} -0.05 \\ -1 \end{bmatrix}.$$

Quantities m_i and λ_i correspond to the magnetization within the segment $[x_{i-1}, x_i]$. Under this notation, the discretization of (4.13) looks as follows

$$\begin{aligned} \tilde{I}(u_{1\dots n}, m_{1\dots n}, \lambda_{1\dots n}) &= \sum_{i=1}^n \frac{1}{2} \langle \mathbb{C}(v_i - \lambda_i v^{01} - (1 - \lambda_i)v^{02}), (v_i - \lambda_i v^{01} - (1 - \lambda_i)v^{02}) \rangle - \\ &- \sum_{i=1}^n (f_i u_i + H_i m_i), \end{aligned} \quad (4.13)$$

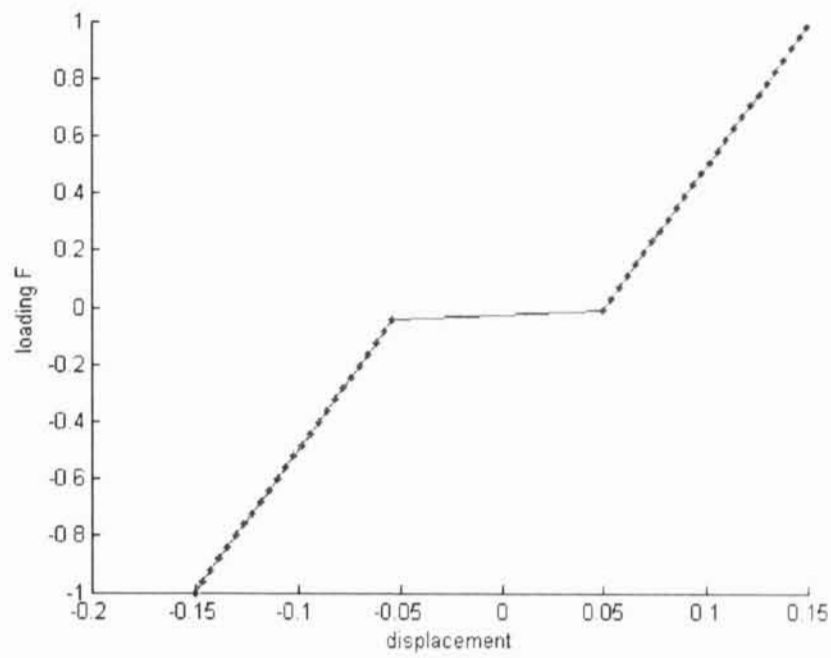
where f_i and H_i stands for $f(x_i)$ and $H(x_i)$, i.e. the external body force and the external magnetic field at point x_i . Notice that we left out the boundary force since in 1D, it may be covered in $F(x_n)$.

To solve this minimizing problem, we use the software MATLAB, which provides the optimization toolbox. Concretely, we take advantage of the function FMINCON, which is designed for finding a minimum of constrained nonlinear multi-variable problem

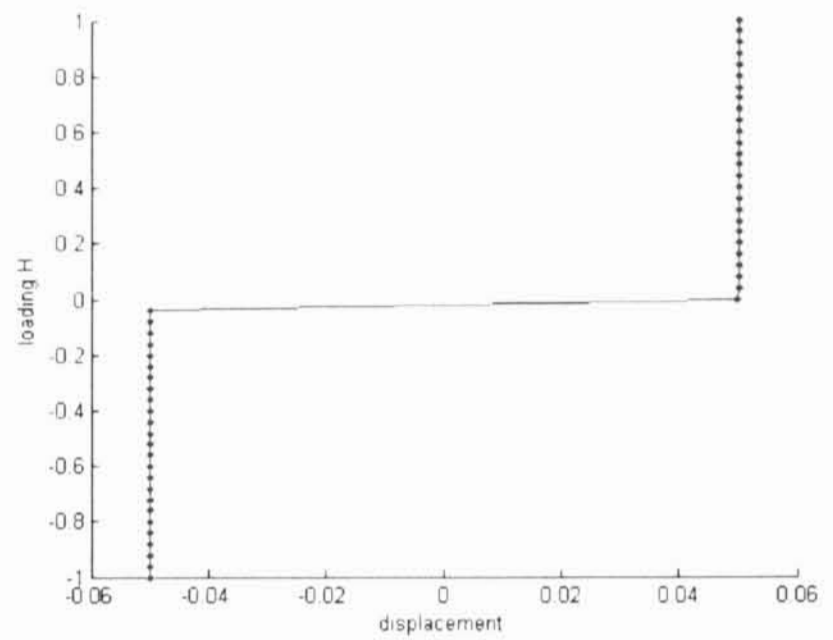
$$\min_x f(x) \quad \text{such that} \quad \begin{cases} c(x) & \leq & 0 \\ ceq(x) & = & 0 \\ A \cdot x & \leq & beq \\ Aeq \cdot x & = & beq \\ lb \leq & x & \leq ub \end{cases},$$

where the right side of the vinculum assigns the constrictions. The functions $c(x)$ and $ceq(x)$ stand for nonlinear constrictions, the matrixes A , Aeq with vectors b , beq give the linear constrictions, and lob and upb defines a set of lower and upper bounds on the design variables in x . In our case, $x = (u_1 \dots u_n, m_1 \dots m_n, \lambda_1 \dots \lambda_n)$ and since we consider homogeneous body loading, we may model the wire as one segment only. So we have $x = (u_1, m_1, \lambda_1)$.

Results we obtain are shown in figures 4.4 - 4.6. Each pair of figures depicts the evolution of one of the variables (u_1, m_1, λ_1) against the loading (strain on the left side and a magnetic field on the right side). The idea of the ferromagnetic shape memory alloys may be easily understood from these plots. Look at the figure 4.4. Since we consider the linear elastic material, the response of the material to the strain is linear, unless it reaches a certain value (in our case unless it changes direction). In this point, it is more convenient for the sample not to remain in its current phase any longer and it jumps over into the second phase. In this phase, the deformation as well as magnetization (see 4.5) are aligned with

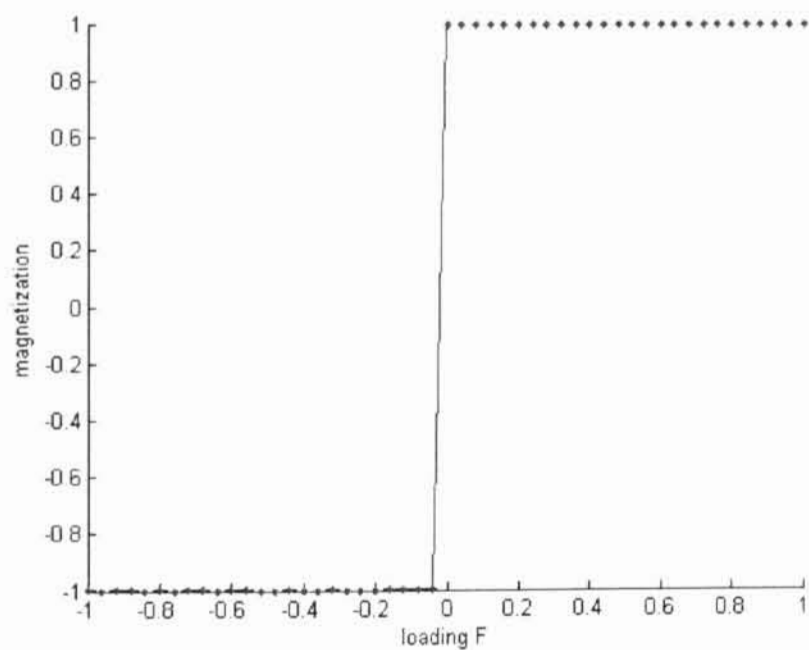


(a) The sample loaded by strain

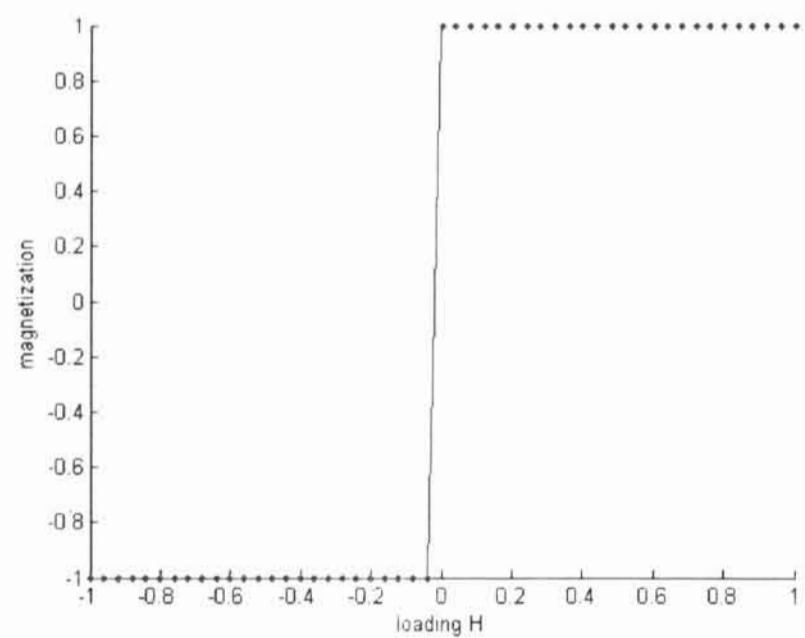


(b) The sample loaded by magnetic field

Figure 4.4: Displacement vs. the external loading fields. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.05$, number of steps 50.

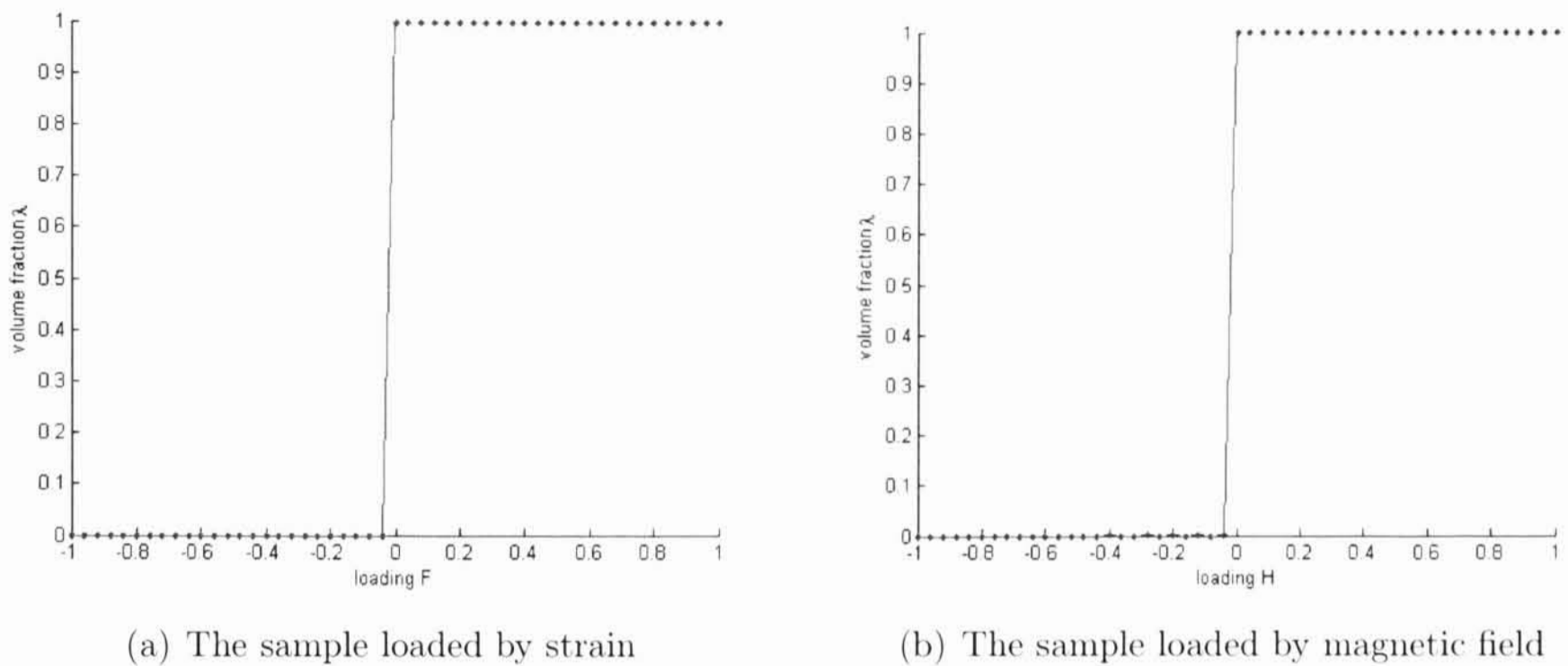


(a) The sample loaded by strain



(b) The sample loaded by magnetic field

Figure 4.5: Magnetization vs. the external loading fields. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.05$, number of steps 50.



(a) The sample loaded by strain

(b) The sample loaded by magnetic field

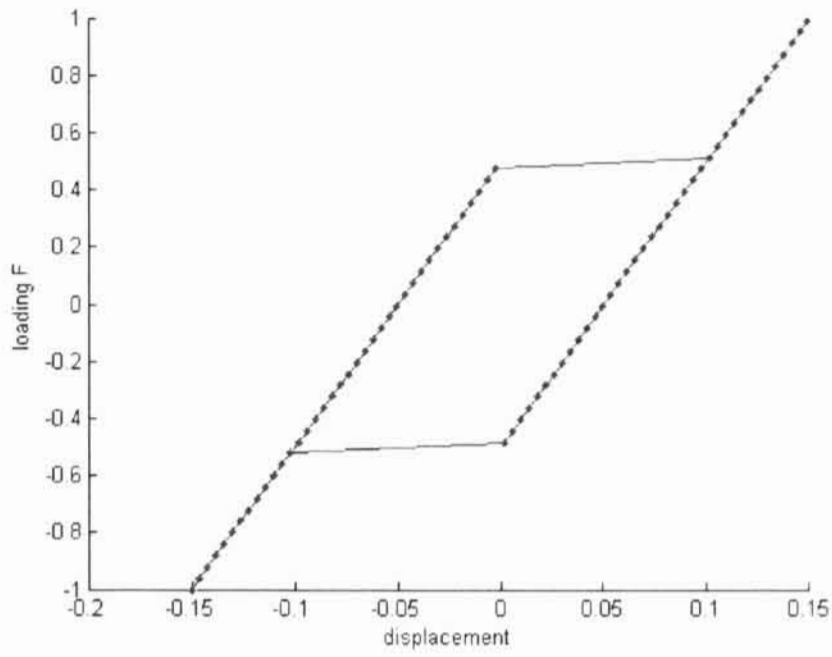
Figure 4.6: Volume fraction vs. the external loading fields. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.05$, number of steps 50.

the loading. The volume fraction fully follows this trend and so for each value of loading, the whole specimen is in only one phase see 4.6).

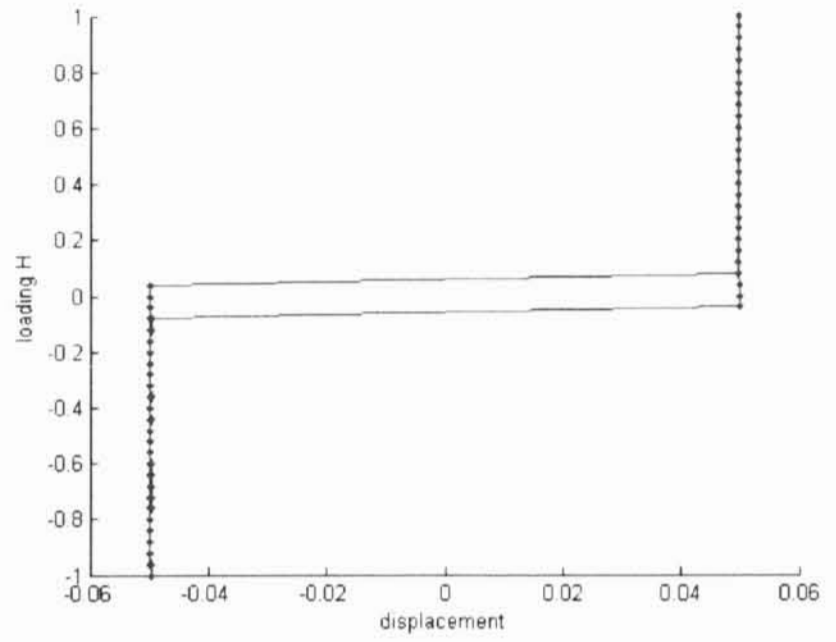
For magnetic active materials it is common to remember state history; that is to say that the state of the specimen is dependent not only on physical properties of its surrounding, but also on the path the sample had to follow to reach the current state. This is usually called hysteresis. To include the effect of hysteresis, slight changes of the energy functional (4.13) need to be done.

$$\begin{aligned}
 \tilde{I}_{hys}(u_{1\dots n}^j, m_{1\dots n}^j, \lambda_{1\dots n}^j) &= \sum_{i=1}^n \frac{1}{2} \langle \mathbb{C}(v_i^j - \lambda_i^j v^{01} - (1 - \lambda_i^j)v^{02}), (v_i - \lambda_i^j v^{01} - (1 - \lambda_i^j)v^{02}) \rangle - \\
 &- \sum_{i=1}^n (f_i^j u_i^j + H_i^j m_i^j) + \sum_{i=1}^n \alpha |\lambda_i^j - \lambda_i^{j-1}|.
 \end{aligned} \tag{4.14}$$

We assume that the loading and so variables vary with equidistant time step. In addition to the i -index, which denotes the position of the point along the wire, the j -index represents certain time step. The added term to (4.14) reflects the tendency of the material to resist the phase change until the energy penalty is too expensive (in terms of energy), the coefficient α scale this property. With respect to work made by Mielke and collaborators in [12], we consider the energy functional to be rate-independent. In the article mentioned above, the time-continues problem is discussed, it is to say the problem with time step $\tau \rightarrow 0$. The existence argumentation for some special nontrivial cases are provided in the same place. The results for the model hysteresis are shown at figures 4.7 - 4.9. We may observe the hysteresis loop caused by a trend described in previous text.

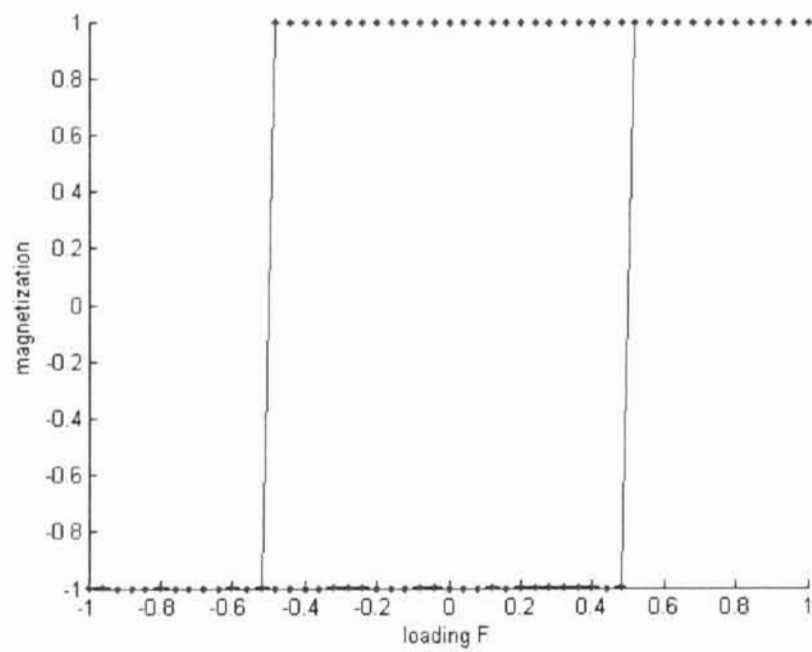


(a) The sample loaded by strain

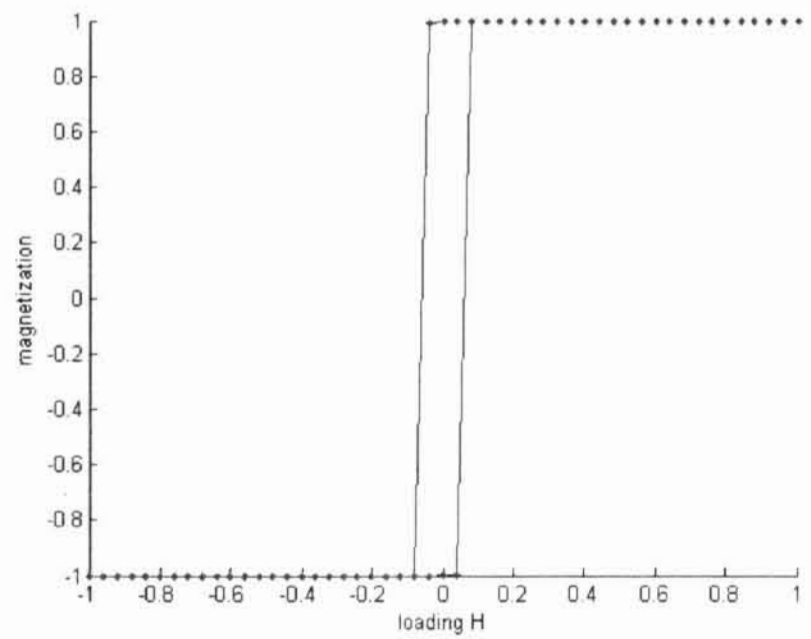


(b) The sample loaded by magnetic field

Figure 4.7: Displacement vs. the external loading fields in model considering the hysteresis. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.1$, number of steps 50.

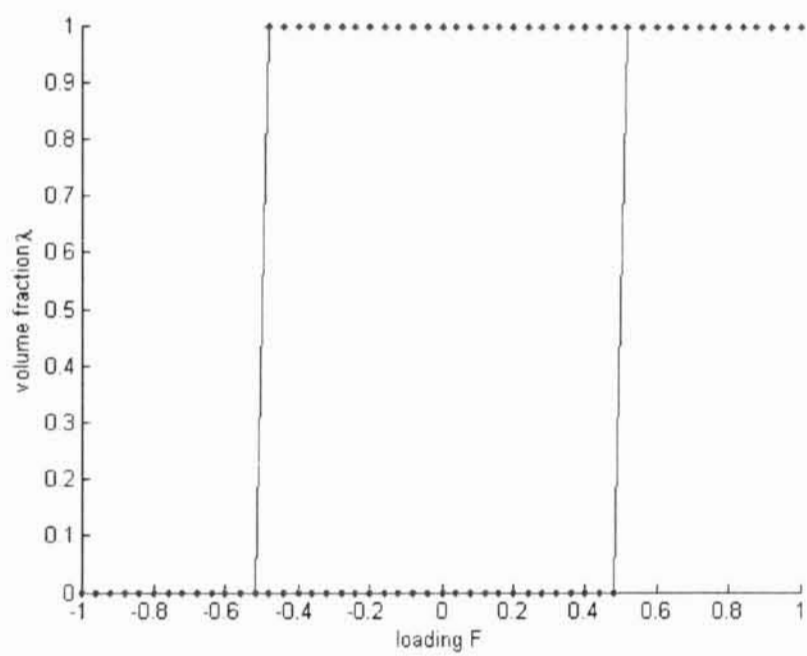


(a) The sample loaded by strain

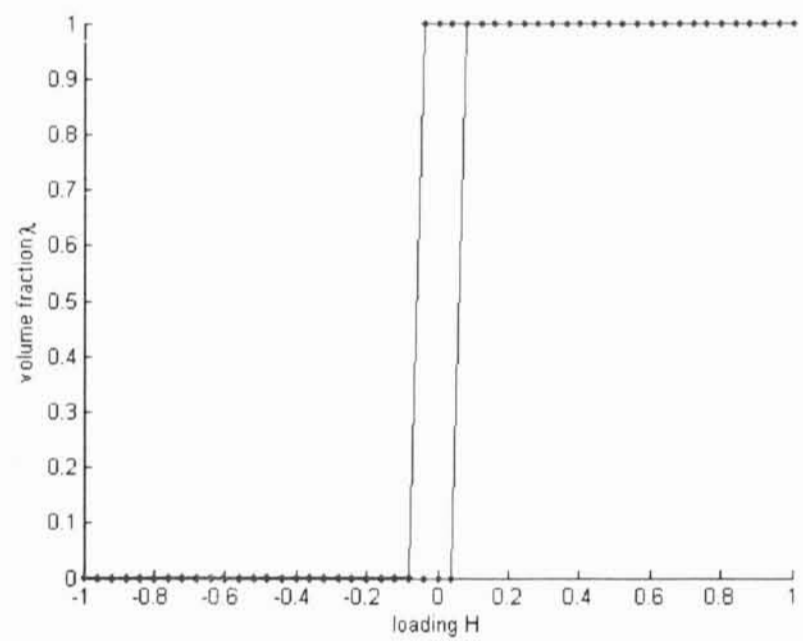


(b) The sample loaded by magnetic field

Figure 4.8: Displacement vs. the external loading fields in model considering the hysteresis. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.1$, number of steps 50.



(a) The sample loaded by strain



(b) The sample loaded by magnetic field

Figure 4.9: Displacement vs. the external loading fields in model considering the hysteresis. Used parameters $\mathbb{C} = \mathbb{I}$, $\alpha = 0.1$, number of steps 50.

Chapter 5

Conclusion

This text focused on describing the phenomena of the ferromagnetic shape memory alloys in terms of mathematical modeling. The theory of linear elasticity and micro-magnetism was studied in order to analyze relevant physical effects and reflect these effects appropriately in a mathematical model. We formulate the potential energy functional of a linear elastic, as well as a ferromagnetic material and combine them with a view to model magneto-elastic behavior.

Our primary goal is not to create a formally faultless model of magnetostrictive material, but we aim to come up with a mathematical description of concerned phenomena with respect to practical usage and numerical implementation (as shown in section 4.3) of the model. Therefore, the problem complexity is shown and afterwards simplifications are introduced with appropriate discussion about potential cost of quality of obtained results. Such a simplification is the usage of the volume fraction λ , which property ($\lambda \in L^\infty(\Omega, \mathbb{R})$) was presumed and which is more of a statistical than a physical value, since $\lambda(x)$ characterizes the surrounding of the point x instead of giving precise information about the behavior directly at point x .

This brings us to the issue, how to potentially extend the work (in accordance with length and quality). One way is to advance in the direction of mathematical theory, study deeply methods of the calculus of variations and introduce more mathematical tools, when dealing with the multiple-well problem, e.g. Young measures approach, see [11]. Another direction may be implementing the 2D model of a ferromagnetic shape memory alloy. This is reasonable and may be useful since it is known that electromagnetic effects take place in the thin surface layer of the sample. And last but not least, process the physical analysis of the model, i.e. assigning physical meaning to the parameters of the mathematical model, calibrating them and preferably verifying the model via comparison with executed experiments.

In conclusion, this thesis lays out the procedure of extending the linear elasticity theory to magnetically active materials. Such a model is then applied to describe a special family of materials - ferromagnetic shape memory alloys. The author is aware of the complexity and complicity of the problem and considers the text as a prologue to a future work.

Appendix A

Used statements

Several important statements were mentioned and used in the text, however no precise formulation was given. Therefore we include these into the Appendix to make the work more comprehensive and transparent. We state Theorems without proof. The reader is supposed to use links referring to individual Theorem. To get more information about Theorem A.0.6 see [15].

Theorem A.0.1 *Let X be a Banach space and let $I : X \rightarrow \bar{\mathbb{R}} = \mathbb{R} \cup +\infty$ be convex and lower semicontinuous, then I is weakly lower semicontinuous.*

Definition A.0.2 *$f : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}$ is said to be quasilinear if f and $-f$ are quasiconvex (see the definition 4.1.3).*

Theorem A.0.3 (The relaxation theorem) *Let $\Omega \subset \mathbb{R}^n$ be a bounded open set with Lipschitz boundary. Let $f : \mathbb{R}^{nm} \rightarrow \mathbb{R}$ be continuous and satisfying*

$$a + \sum_{i=1}^N b_i |\Phi_i(A)|^{\beta_i} \leq f(A) \leq c + \sum_{i=1}^N d_i |\Phi_i(A)|^{\beta_i}$$

for every $A \in \mathbb{R}^{nm}$ and for some $a, c \in \mathbb{R}$, $N \geq 1$, $\beta_i > 1$, $d_i \geq b_i > 0$ and where $\Phi_i : \mathbb{R}^{nm} \rightarrow \mathbb{R}$, $i = 1, \dots, N$ are quasilinear. Let $u \in W^{1,\infty}(\Omega, \mathbb{R}^m)$, then there exists $\{u^s\}_{s=1}^\infty$, $u_s \in W^{1,\infty}(\Omega, \mathbb{R}^m)$ such that

- i) $u^s = u$ on $\partial\Omega$,*
- ii) $\Phi_i(\nabla u^s) \rightarrow \Phi_i(\nabla u)$ in $L^{\beta_i}(\Omega)$, $i = 1, \dots, N$, as $s \rightarrow \infty$,*
- iii) $\int_\Omega f(\nabla u^s(x)) dx \rightarrow \int_\Omega Qf(\nabla u(x)) dx$ as $s \rightarrow \infty$,*

where Qf is quasiconvex envelope of f .

Definition A.0.4 Let X^* be dual space to normed vector space X over \mathbb{R} (or \mathbb{C}) and X^{**} be dual space to Banach space X^* . We define continuous linear transformation $\kappa : X \rightarrow X^{**}$

$$\kappa_f(x) = f(x) \quad \forall x \in X \text{ and } f \in X^*.$$

Since mapping κ preserve the norm, it is injective. The space X is called reflexive, if κ is bijective.

Theorem A.0.5 (Equivalent definition of reflexive space) Let X be a Banach space, then the following are equivalent

1. The space X is reflexive.
2. The dual space of X is reflexive.
3. Every bounded sequence in X has a weakly convergent subsequence.
4. Every continuous linear functional on X attains its maximum on the closed unit ball in X .

Theorem A.0.6 Let $\Omega \in \mathbb{R}^n$ be a bounded set with Lipschitz boundary, $p \in \langle 1, n \rangle$, then

$$\forall q \in \langle 1, p^* \rangle \quad W^{1,p}(\Omega) \hookrightarrow L^q(\Omega),$$

where $p^* = \frac{pn}{n-p}$.

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