STUDY OF THE INFLUENCE OF EDGE PROFILES OF PERMALLOY (Ni$_{80}$Fe$_{20}$) NANOWIRES ON THE MAGNETIC BEHAVIOR OF DOMAIN WALLS USING MICROMAGNETIC SIMULATIONS

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A Dissertation Submitted to the Department of Physics, Bangladesh University of Engineering & Technology, Dhaka in Partial Fulfillment of Requirement for the Degree of Master of Philosophy in Physics

SUBMITTED
By

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Dedication

To my mother
CANDIDATE’S DECLARATION

This thesis is a presentation of my original research work. Wherever contributions of others are involved, every effort is made to indicate this clearly, with due reference to the literature, and acknowledgement of collaborative research and discussions. The work was done under the guidance of Dr. Mohammed Abdul Basith, at the Department of Physics, Bangladesh University of Engineering & Technology, Dhaka, Bangladesh.

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Abstract

Understanding and controlling of domain wall (DW) behavior in patterned ferromagnetic nanowires are crucial for their potential applications in proposed digital logic and memory devices. For the operation of a memory, logic or sensing device, firstly well-defined domain walls are necessary and secondly a precise control in the domain walls movement is required. Previous investigations demonstrated that trapping sites such as notch or anti-notch of different geometries allow control of the position of DWs in ferromagnetic nanowires. Magneto-optic Kerr effect magnetometry, off-axis electron holography and magnetic imaging techniques have contributed useful information for a greater understanding of the behavior of DWs in nanowires. Since many years, micromagnetic simulations have also been playing a significant role to understand the controlled behavior of DWs in ferromagnetic nanowires. So far to simulate the behavior of the DWs along nanowires, a standard rectangular cross-section of the wire edge (referred as rectangular/vertical wire edge) was considered. But patterning of nanowires by using advanced nanofabrication techniques like electron-beam lithography and focused ion beam milling and their cross-sectional images recorded by using transmission electron microscope demonstrated that the wire edge of the patterned nanowires is either sloped or tapered rather than rectangular (vertical). Therefore, in the present investigation by using micromagnetic simulations we have studied the influence of standard rectangular and experimentally observed edge profiles of Permalloy ($\text{Ni}_{80}\text{Fe}_{20}$) nanowires on the magnetic behavior of DWs. We have observed the energy minimization in nanowires which were modeled based on experimentally observed sloped and tapered edge profiles compared to that of rectangular edge profiles. The domain wall depinning field from anti-notch which actually indicates the strength of the pinning potential was found to increase if the edge profile of the nanowires is also sloped or tapered rather than rectangular. The sloped or tapered edges certainly have an affect due to the effective variation of nanowire width. In the case of vortex domain wall, we also believe that nucleation of wall also affects for example the vortices also changes
significantly with the sloped or tapered edge compared to the flat rectangular (vertical) edge. The domain wall structure was found to extend significantly prior to depin from the anti-notch if the edge profile of the modeled nanowires is rectangular. Notably, such an extension of the wall structure is either absent or reduced if the edge profiles are modeled following the experimentally observed profiles of the patterned nanowires. The unmodified wall structure prior to depin from the anti-notch is highly expected to realize the proposed DW based nanowire devices. This is due to the fact that the size of the domain walls governs the achievable miniaturization and thus the data storage density. The total energy as a function of normalized magnetization, depinning field strength, interaction mechanism of DWs with anti-notch and most importantly the wall structure prior to depin from the anti-notch were reported in this investigation. Finally the consequences of our findings were noted and a definition of the experimentally observed edge profiles of the nanowires was highlighted for a reliable operation of the future logic and memory devices.
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Chapter 1

Introduction

1.1 Introduction

Understanding and controlling of domain wall (DW) behavior in patterned ferromagnetic nanowires are crucial for their potential applications in proposed digital logic and memory devices [1–4]. In magnetic field driven nanowire devices, information is encoded in the magnetic states of domains and domain wall motion along the wires allows for the access and manipulation of the stored information. Therefore, a precise control of the DW motion along the nanowires is required prior to realize the device applications [1–5]. In a domain wall (Néel type), the magnetization direction gradually changes from one domain to the other within the plane of the magnetic film. In soft magnetic structures like Permalloy ($Ni_{80}Fe_{20}$) nanowires, the magnetization direction is restricted parallel to the wire axis because of the large shape anisotropy, figure 1.1. Therefore, the spin structure of domain walls in these nanowires depends on the element width and thickness. Nakatani et al. [6] have established a refined phase diagram by numerical calculations and found different domain wall spin configurations like vortex and transverse types which are energetically favorable for certain element widths and thicknesses. These magnetic configurations are characterized by their axial magnetization alignment, which can be either head-to-head or tail-to-tail
depending on the magnetization pointing towards or away from the wall, respectively.

The transverse wall comprises of, to first approximation, two 90° walls with the spin in the central domain perpendicular (magnetization pointing either up or down) to the wire axis, figure 1.2(a). The vortex domain wall consists of three distinct wall sections where the magnetization rotates about a central vortex core, an out-of-plane magnetization component. A vortex wall is also identified by the vortex chirality, which can be clockwise or counter clockwise depending on the sense of spin rotation about the vortex core, figure 1.2(b). Previous investigations demonstrate that trapping sites such as notch or anti-notch of different geometries allow control of the position of DWs in ferromagnetic nanowires [2–15]. Magneto-optic Kerr effect magnetometry [10, 16], off-axis electron holography [17], and magnetic imaging techniques [5, 11, 12, 18] have contributed useful information for a greater understanding of the behavior of DWs in nanowires. Since many years, micromagnetic simulations [4, 6–8, 19] have also been playing a significant role to understand the controlled behavior of DWs in ferromagnetic nanowires. So far to simulate the behavior of the DWs along nanowires, a standard rectangular cross-section of the wire edge (from now referred as rectangular edge profile) was considered. But patterning of nanowires by using advanced nanofabrication techniques like electron-beam lithography [5], and focused ion beam milling [9, 12], and their cross-sectional images recorded by using transmission electron microscope demonstrated that the wire edge of the patterned nanowires is either sloped or tapered [9, 14], rather than rectangular. Till date to the best of our knowledge, there is no published information on the detailed way in which the behavior of DWs changes with applied magnetic field by varying the edge profile of the nanowires. Therefore, in the present investigation by using micromagnetic simulations we intend to study the influence of standard and experimentally observed edge profiles of Permalloy ($\text{Ni}_{80}\text{Fe}_{20}$)
nanowires in the magnetic behavior of DWs. In particular, we are interested to compare the properties like the total energy as a normalized magnetization, their depinning field strength and interaction mechanism with anti-notch by considering DWs of different structures along nanowires of standard and experimentally observed edge profiles. The structures of the DWs like transverse up (TUP), clockwise vortex (CWVDW) and counter-clockwise vortex (CCWVDW) will be considered by varying the width of the nanowires with a fixed Permalloy film thickness as was suggested in the DW structure phase diagram [6]. The motivation of this investigation is described in the next section.

1.2 Motivation

The recent advancement in nanofabrication technology opens fascinating opportunity for engineering innovative magnetic materials and pushes the dimension of ferromagnetic structure into nanoscale where the structure dimensions become comparable to certain characteristics length scales, such as exchange length or the domain wall width [2, 20, 21]. At the nanoscale the magnetic properties of ferromagnetic materials are governed by the geometry of the material in addition to the intrinsic material properties. Therefore, it is possible to engineer the geometry to tailor the domain wall spin structure and switching behavior of the patterned nano elements (in the present investigation this is ferromagnetic nanowire). This is particularly true in the case of soft magnetic materials like Py where the effect of magnetocrystalline anisotropy is small. Magnetic DWs in these patterned nanowires can be manipulated using external magnetic fields [7, 22–29] and spin polarized currents [30–34].

Therefore, a precise understanding and control of magnetic DWs in the patterned ferromagnetic nanostructures is of recent fundamental scientific interest due to their promising applicability in future spintronic devices such DW logic [1, 2, 35–37] and racetrack memory [3, 38, 39]. In a logic device the magnetic domain wall will be utilized as a mobile interface between two oppositely magnetized domains. The domains themselves form the basis of a binary information representation, whereby a logical "1" and "0" are represented by the magnetization within two oppositely magnetized domains. Major advantage of using domain walls in such a logic architecture include the
production of low power high speed, and low cost devices for next generation computing technology. Another promising application of magnetic DWs is to store information in three dimensional structures called race-track memory system [3]. The new class of future memory device will promise features such as high performance, low cost and non-volatility. Short pulses of spin polarized currents are used to move domain walls (DWs) between pinning sites. Arrays of nanowires can be used to form the racetrack device where these nanowires can be placed horizontally or vertically, figures 1.3A and 1.3B. A single bit data can be stored in DWs between two successive magnetic regions, which can be differentiated by the direction of local magnetization, or by presence and absence of DWs between two regions. Many DWs (as many as 10-100) can be stored in a single racetrack. As a result, the stored number of data bits per unit area can be increased dramatically compared to the conventional 2D random access memories (RAM based technologies). This ultimately demand a precise control of the DW mo-
tion along the nanowires prior to realize the device applications [2–5]. As a part of the upsurge in global research interest in patterned ferromagnetic nanowires, using high resolution magnetic imaging techniques and micromagnetic simulations researchers have contributed useful information to understand the fundamental properties and behavior of DWs in the patterned Permalloy ($\text{Ni}_{80}\text{Fe}_{20}$) nanowires. Key questions of these investigations were - how can DWs in the patterned nanowires be reproducibly nucleated [5, 8, 11] How does the pinning potential of geometrical features such as notch/anti-notch interact with DWs to identify precisely the location of the DWs [4, 5, 7, 9–11]. An important consideration which was not investigated comprehensively is the influence of nanofabrication techniques on the re-producible nucleation and propagation of DWs in the fabricated nanowires. It is noteworthy that to ensure the reliable operation of the proposed ferromagnetic devices by reducing the performance variability, high quality nanofabrication is extremely important. Previous reports [40–43] indicate that the structural roughness at the edges of the nanowires produced by fabrication processes affect the magnetic properties of the nanostructures. Some recent rare investigations using high resolution TEM cross-sectional imaging technique clearly demonstrated that the edge profiles of the patterned nanowires are varied [9, 14] and these are distinct notably from ideal consideration (this is described elaborately in section 3.4 of chapter 3). This actually motivated us to investigate the influence of edge profiles of the patterned nanowires on the magnetic behavior of domain walls by using a widely used simulation package ‘Object Oriented Micromagnetic Framework’ (OOMMF) developed by National Institute of Standard and Technology (NIST), USA [19]. In the next section the objective of this investigation is described precisely.

1.3 Objectives

The main objectives of the present research are as follows:

(1) Modeling of the Permalloy nanowires of standard rectangular shape edge profile and also experimentally observed sloped and tapered edge profiles. Variation of width of the nanowires from 100 nm to 300 nm for a fixed 10 nm thickness of Py following to DW structure phase diagram [6] to create transverse and vortex

Section 1.3
types of DWs.

(2) Simulation of the DW nanostructures by using a widely used and freely available code, Object-Oriented Micromagnetic Framework (OOMMF) developed by Information Technology Laboratory of National Institute of Standard and Technology (ITL/NIST), USA [19].

(3) Designing initial DW structures at the left side of the nanowire by creating color coded magnetic regions and relaxing it to its ground energy state. Initiating DW movement by applying magnetic field towards the direction of the anti-notch in step by step fashion.

(4) Investigation of the total energy as a function of normalized magnetization and their field strength of DWs for various wall structures along nanowires of varying edge profiles.

(5) Investigation of the interaction mechanism of the DWs with geometrical feature, anti-notch in the nanowires of varying widths and edge profiles.

(6) Evaluation of the domain wall configurations prior to depin from the anti-notch.

1.4 Organization of the thesis

Chapter 1.1 presents an introduction as well as motivation of this investigation. This chapter introduces the background for domain walls in magnetic nanowires with an emphasis on nanowire based devices. Chapter 2 describes basic ferromagnetism, micromagnetic energy terms, domain wall configurations and their observation techniques. Micromagnetics simulation including the geometry of the edge profiles of the nanowires, materials parameters etc. are illustrated in Chapter 3. Domain wall pinning studies at symmetric and asymmetric anti-notch of nanowires by varying their edge profiles are described in Chapter 4. The summary of this investigation and an insight of future works were presented in Chapter 5.
Chapter 2

Background

This chapter presents an overview of magnetism, particularly basic ferromagnetism. The micromagnetic energy terms, basic concepts of magnetic domains and domain walls, the observation technique of domain walls etc. were described in this chapter.

2.1 Basic concept of ferromagnetism

The origin of magnetism lies in the orbital and spin motions of unpaired electrons and how the electrons interact with one another. Therefore, magnetic properties of materials are mainly restricted to compounds of transition metals and lanthanides, many of which possess unpaired d or f electrons. In all other materials, electrons are paired in their orbitals with opposite spin and their magnetic effects cancel. These type of materials are known as diamagnetic materials. The class of materials in which atoms or ions have a net magnetic moment due to unpaired electrons in partially filled orbitals is known as paramagnetic. Without an external magnetic field, magnetic moments are randomly oriented and thus they mutually cancel one another. As a result, like diamagnetism, the net magnetization in these materials is zero, figure 2.1 (a). However, when an external field is applied the individual magnetic vectors tend to turn into the field direction.

Ferromagnetism is a phenomenon by which a material can exhibit a spontaneous magnetization below a critical temperature named as Curie temperature \( T_c \) and is responsible for most of the magnetic behaviour encountered in everyday life. In ferro-
magnetic materials, the spontaneous magnetization varies with temperature, and has a maximum value at 0 K and is reduced to zero at the $T_c$ as shown in figure 2.2. In a particular class of ferromagnetic materials, instead of a parallel alignment of all the spins, there can be an anti-parallel alignment of unequal spins as shown in figure 2.1 (c).

![Figure 2.1: Schematic diagram of the alignment of magnetic moments in (a) paramagnetic, (b) ferromagnetic, (c) ferrimagnetic and (d) antiferromagnetic specimens.](image)

This also results in a spontaneous magnetization, which is known as ferrimagnetism. On the other hand, antiferromagnetic materials exhibit, just as ferromagnetics, spontaneous alignments of moments below a critical temperature. However, the responsible neighbouring atoms in antiferromagnetics are aligned in an antiparallel fashion and hence the net magnetic moment is zero, figure 2.1 (d). The mechanism for the appearance of spontaneous magnetization in ferromagnetic materials was first clarified by P. Weiss in 1907 [44]. Weiss postulated that the magnetic moment of the individual electrons (or atoms) interact with each other and possess a spontaneous magnetization in the absence of an applied magnetic field. Weiss described the origin of this interaction
in the form of an internal molecular field, $B_m$, which is proportional to the spontaneous magnetization.

$$B_m = \lambda M$$  \hspace{1cm} (2.1)

where $\lambda$ is known as the molecular field coefficient. Heisenberg later explained the nature of this field in the quantum mechanical exchange effect, and is described by the Heisenberg exchange Hamiltonian,

$$H_{ij} = -2J s_i s_j$$  \hspace{1cm} (2.2)

where the $H_{ij}$ is the exchange energy of two interacting electron spins ($s_i$ and $s_j$) and $J$ is the exchange integral, which is dependent on the material. If the exchange integral in ferromagnets is positive, that causes a minimum energy for parallel spins. The antiferromagnets have a negative exchange integral resulting in a minimum energy when the spins are antiparallel. The exchange energy is discussed further in section 2.2 along with other energy terms.

### 2.1.1 Ferromagnetic material Permalloy ($Ni_{80}Fe_{20}$) and it’s technological application

In the early 20th century a remarkable magnetic alloy was discovered in the Bell System Laboratory that contain nickel and iron. These alloys are the most versatile of all magnetic materials for electromagnetic applications. The most startling results are obtained with alloys of approximately 80 percent nickel and 20 percent iron [45], whose permeabilities at small strengths are many times greater than any hitherto known. The alloys of this approximate composition was given the name ”Permalloy” (Py) [45]. The Py with a composition of $Ni_{80}Fe_{20}$, today is a well known soft magnetic alloy, forms a face-centered-cubic structure. Soft magnetic materials like Py are best suitable for application in memory devices and sensor technology because they are easy to magnetized and demagnetize. Due to high permeability, high saturation magnetization also near zero magnetostriction and zero crystal anisotropy the domain wall movement in Py is easy and require much less energy. So, much denser domain can be formed for
high density spintronic memory devices and magnetic logic gates [35, 36].

In this investigation we have studied domain walls behavior in soft Py nanowires by varying the edge profiles of the nanowires.

### 2.2 Micromagnetic energy terms

The exchange interaction described earlier cannot explain alone the ferromagnetic behavior and there are other energy contributions that must be taken into account. A number of different competitive micromagnetic energy terms contribute to the total energy of a ferromagnetic specimen. A stable state is reached when the micromagnetic energy is locally minimised. These energy terms are discussed as follows.

#### 2.2.1 Exchange energy

The exchange energy is the energy associated with the parallel alignment of the spin system. Heisenberg’s model [46] suggested the origin of ferromagnetism was due to the exchange interaction when the wave functions of two neighboring electrons overlap.

The energy in a ferromagnetic sample is given by:

\[
E_{ex} = -2JS^2 \sum \cos \phi_{ij}
\]  
(2.3)

where \( S \) is the magnitude of the spin, \( \phi_{ij} \) is the angle between spins \( i \) and \( j \), and \( J \) is the exchange integral. Taking into account the three dimensional nature of crystals and integrating over a finite volume of the material (in the simple case for a cubic system), the exchange energy simply written as:

\[
E_{ex} = A \int_V [(\nabla \alpha)^2 + (\nabla \beta)^2 + (\nabla \gamma)^2] dV
\]  
(2.4)

here, \( \alpha, \beta, \gamma \) are the direction cosines with respect to the crystal axes, and \( A \) is the exchange stiffness constant of the material, which is given by (for cubic system):

\[
A = \frac{kJS^2}{a}
\]  
(2.5)
with $k$ is a structure-dependent constant (1 for simple cubic, 2 for body centered cubic and 4 for face-centered cubic crystals) and $a$ is the lattice parameter. For example, exchange stiffness constant for permalloy ($Ni_{80}Fe_{20}$) is $A = 13 \times 10^{-12} J/m$ [47]. Normally, exchange energy is minimized in magnetic domains because of parallel alignment of the magnetic moments in the domains. However, in magnetic domain walls, the exchange energy becomes significant because the magnetic moments in the wall deviates from one direction to another one over the wall width.

### 2.2.2 Anisotropy energy

Anisotropy energy is related to the directional behaviour of the materials, in which the magnetization properties depends on the measuring direction because the orientation of the magnetization is influenced by the structure of the materials. There are two main types of anisotropy: magnetocrystalline and shape anisotropy (demagnetising energy).

**Magnetocrystalline Anisotropy**

The magnetocrystalline anisotropy is caused by the spin-orbit interaction. The electron orbits are linked to the crystallographic structure, and the spin orbit interaction gives non-spherical charge distribution, that results in a preferred orientation direction of magnetization. The preferred directions for magnetization are called the easy axis and the directions in which it is most difficult to align the magnetization are called hard axis. Magnetocrystalline anisotropy is associated with the energy necessary to deflect the magnetic moment in a single crystal from the easy to the hard direction. For a hexagonal system, there is a uniaxial anisotropy with the energy given by [48]:

$$E_k = \int_V (K_1 \sin^2\theta + K_2 \sin^4\theta) dV$$  \hspace{1cm} (2.6)

where, $\theta$ is the angle between the magnetization and easy axis, $K_1, K_2$ are first and second magnetocrystalline anisotropic constants, respectively. For example, $K_1 = 4.1 \times 10^5 J/m^3$, $K_2 = 1.5 \times 10^5 J/m^3$ for Co. If we use the direction cosine, 2.6 becomes:

$$E_k = \int_V [K_1(1 - \gamma^2) + K_2(1 - \gamma^2)^2] dV$$  \hspace{1cm} (2.7)
In the case of polycrystalline materials there is no overall preferred axis for magnetization because the crystallites are randomly oriented. Instead, the anisotropy direction varies from crystallite to crystallite, i.e. local easy axes. Additionally, induced anisotropy can be created during or after growth process of the film using special treatment techniques [48].

**Shape Anisotropy**

The shape anisotropy is related to the magnetostatic effects of the system rather than the overlap of electron orbitals, however, it is specially important to the magnetic configurations of the thin films and objects with reduced dimensions. When a magnetic specimen is uniformly magnetised, the magnetic free poles are present at the surface of the specimen. Figure. 1.3 illustrates that the magnetostatic dipole interactions may produce magnetic anisotropy in an ellipsoid specimen magnetised along the long and short axes, it can be seen that free poles are separated by relatively long and short distances respectively. Inside the specimen with ellipsoid shape (figure 2.3), the demagnetising field, $H_d$, is aligned oppositely to the direction of the magnetization and the shape anisotropy energy will be given by [48]:

$$E_k = \int_V K_{\text{eff}} \sin^2 \theta dV$$

(2.8)

here,

$$K_{\text{eff}} = \frac{(N_b - N_a) M^2}{2}$$

(2.9)

where, $\theta$ is the angle between the long axis and the magnetization direction, $M$ is the magnetization, and $N_a, N_b$ are demagnetising factors in the long and the short axes, respectively. The demagnetising factors depends on the sample geometry and in 3D

Section 2.2
case, the demagnetising factors in the three dimensions are given by:

\[ N_a + N_b + N_c = 1 \quad (\text{in SI unit}) \quad (2.10) \]

### 2.2.3 Magnetostatic energy

Inside a magnetic specimen, the magnetic induction \( B \) is expressed as:

\[ B = \mu_0 (H + M) \quad (2.11) \]

where \( \mu_0 \) is the permeability of free space, \( H \) is the magnetic field strength and \( M \) is the magnetization of the uniformly magnetized specimen. Using this relationship, the divergence of \( M \) can be expressed as:

\[ \nabla \cdot M = \frac{\nabla \cdot B}{\mu_0} - \nabla \cdot H \quad (2.12) \]

From Maxwell’s equation,

\[ \nabla \cdot B = 0 \quad (2.13) \]

Therefore,

\[ \nabla \cdot H = -\nabla \cdot M \quad (2.14) \]

This non-zero divergence of magnetization at the sample surface and also from within volume of the material give rise to field \( H \) that ensure the continuity of lines of \( B \). This field is known as the demagnetizing field or magnetostatic field or stray field \( H_d \).

Therefore, we can write:

\[ \nabla \cdot H_d = -\nabla \cdot M \quad (2.15) \]

Magnetostatic energy effects arise from any magnetization distribution which results from the build up of magnetic charge at the surface of a magnetic specimen and also from within a volume when the magnetization distribution is discontinuous or divergent. As mentioned above, these poles generate a field which exists both inside (demagnetizing field) and outside (stray field) the specimen, with \( H_d \) opposing the magnetization. The magnetostatic energy in the SI unit will be given by:
Figure 2.4: The magnetic field generated by a field source at the point P: due to surface magnetic charge and volume magnetic charge from a point $r'$

\[ E_d = -\frac{\mu_0}{2} \int_V \mathbf{M} \cdot \mathbf{H}_d dV \] (2.16)

with $\mu_0$ is the permeability of free space. The magnetostatic field, $\mathbf{H}_d$ at a point $P$ at a position $\mathbf{r}$ to the origin of the coordinate $(O)$ originates from the surface $(S)$ and the volume $V$ charges (see 2.4), represented by [49]:

\[ \mathbf{H}_d = -\frac{1}{4\pi} \int_V' \frac{\nabla \mathbf{M}}{|\mathbf{r} - \mathbf{r}'|^2} dV' + \frac{1}{4\pi} \int_S' \frac{\mathbf{M} \cdot \mathbf{n}}{|\mathbf{r} - \mathbf{r}'|^2} dS' \] (2.17)

where $\mathbf{r}$ is the position vector for the point at which the field from the magnetic charge is evaluated, $\mathbf{r}'$ is the position of the differential magnetic charge. The magnetostatic energy of the specimen can be reduced by decreasing the amount of stray field generated at the edges or within the specimen. This can be achieved by the formation of the domain structure 2.3.

### 2.2.4 Zeeman energy

When the specimen is placed in an external field, the magnetic moments within the specimen will tend to align parallel to the applied field. The Zeeman energy takes into account the orientation of the magnetization with respect to the applied field and is
given by:

\[ E_z = -\mu_0 \int_V \mathbf{M}.\mathbf{H}dV \] (2.18)

where \( \mu_0 \) is the permeability of free space.

### 2.2.5 Magnetostrictive energy

Magnetostrictive energy is associated with materials in which the dimension of a ferromagnet is changed when subjected to an external magnetic field. Conversely, the magnetization of the ferromagnet will be varied when it is exerted by a stress. As a result, the magnetostrictive energy term is written as [48]:

\[ E_\lambda = \int_V \frac{3}{2} \lambda \sigma \sin^2 \alpha dV \] (2.19)

where \( \alpha \) is the angle between saturation magnetization and the stress, \( \sigma \). The \( \lambda_s \) is the saturation magnetostriction of the material, e.g. \( \lambda_s = -0.2 \times 10^{-6} \) for \( Ni_{80}Fe_{20} \) polycrystalline film [50]

The magnetostrictive energy is originated from spin-orbit interaction in ferromagnetic materials. The magnetostriction occurs when the electron cloud is not is spherically symmetric shape and has strong spin-orbit interaction. Under an applied magnetic field, the orbital moment tends to align with the field and distort the orbit. This effectively alters the position of the atom within the material and creates mechanical strain. The specimen either expands (positive magnetostriction) or contracts (negative magnetostriction) in the direction of the magnetization.

### 2.2.6 Total energy

The total energy of a ferromagnetic specimen is the sum of the individual energy terms which are described above:

\[ E_{total} = E_{ex} + E_k + E_d + E_z + E_\lambda \] (2.20)
and the magnetic configuration (domain structure, which will be discussed in the next section) is a direct consequence of its local or global minimization.

2.3 Magnetic Domain and Domain Configurations

In ferromagnetic materials, the spins of unfilled d-bands spontaneously align parallel to each other below Curie temperature $T_c$, i.e. they align within small domains without the presence of an external magnetic field. The theory behind the formation of this domain structure has been given by Landau and Lifshitz [51] who showed that the sub-division of a specimen into domains could result in a considerable reduction in the magnetostatic energy from that of the saturation condition, albeit at the cost of an increase in exchange energy. Therefore, understanding the magnetic domain configuration and domain wall structure is crucial for micromagnetic investigations.

Weiss first established the concept of magnetic domains [44]. A magnetic domain is a region in which the magnetic moments align parallel. The existence of magnetic domains was indirectly confirmed at first by the detection of the Barkhausen jump [52] in the magnetization curve, in which the reorientation of domains caused discrete changes in the magnetic induction within a ferromagnetic specimen which could be probed by a suitable amplification of the signal from a search coil wound around the specimen. The second confirmation, and the first direct visualization was the observation of magnetic domain patterns on the surface of a ferromagnetic material by Bitter [53]. In the experiment, Bitter used a suspension solution made of the fine magnetic powder suspended in a carrier liquid which was spread on the surface of the specimen. The domain patterns were observed in the particle accumulations when viewed under an optical microscope. The formation of the magnetic domains was subsequently explained in theory by Landau and Lifshitz [54, 55] and then developed by Kittel et al. [56]. Later micromagnetic theory established by William Fuller Brown Jr. in 1963 [57], explained the existence of domains as a consequence of the micromagnetic energy minimization. For example, a breakup of the magnetization into localized regions (magnetic domains) providing for flux closure at the ends of the specimen, reduces the magnetostatic energy. It is provided that the decrease in magnetostatic energy is
greater than the energy necessary for forming domain walls then multi-domain patterns will arise. Some examples can be referred to Figure. 2.5: strong uni-axial anisotropy.

![Diagram of domain wall configurations](image)

Figure 2.5: Variation of domain structure in a square thin film element: a) single domain cubic, b) multi-domain state with large magnetostatic energy, c) magnetocrystalline anisotropy, d) anisotropic flux closure, e) single-domain shape anisotropic state in a rectangular element, f) S-state in the rectangular.

cubic square patterned film with large stray field (a), multidomain in uni-axial square to reduce stray field, and magnetostatic energy but increasing exchange energy (b), flux-closed square patterned soft magnetic thin film without stray field, no magnetostatic energy (c), weak uni-axial anisotropy with reduced magnetostatic energy (d), single-domain strong shape anisotropy with stray field and magnetostatic energy (e) and multi-domain shape anisotropy with reducing magnetostatic energy (f).

The configurations with non-global minimization are called meta-stable states and are the local minimization for the system. The configuration supported by a sample depends on the magnetization history of the material as well as the strength and direction of the applied magnetic field. Applying a particular field will usually vary the configuration from one state to another.

### 2.3.1 Domain wall configurations

A magnetic domain wall is identified by its spin configuration and the angle through which the magnetic moments rotate from one domain to the next one. There are basically two types of domain wall: Bloch-type wall (a) and Néel-type wall (b)(Figure. 2.6. In the Néel wall, magnetic moments gradually rotates in plane of the film whereas in the Bloch wall, the magnetic moment rotation is out-of-plane. There is no divergence...
of the magnetization for the Bloch wall. Hence, the Bloch walls are favorable in the thick film (\(>90\text{nm}\)) in which the associated stray field is small. Taking into account the different energy terms, the width of a Bloch domain wall only depends on the exchange and magnetocrystalline anisotropy.

\[
\delta_B = \pi \sqrt{\frac{A}{K_1}}
\]  

(2.21)

Here, \(A\) and \(K_1\) are the exchange constant and magnetocrystalline anisotropy constant of the material, respectively. For example, the Bloch wall width of iron is \(\delta_B \approx 40\text{nm}\) \([58]\). Whereas, in the thin film, the out-of-plane magnetization intersects the surface, free poles are created, therefore, the Bloch wall may become unfavorable. Instead the Néel wall structure occurs. The width of a Néel wall is dependent on the exchange energy.

![Schematic illustration of (a) Bloch-type, (b) Néel-type wall and (c) cross-tie wall](image)

Figure 2.6: Schematic illustration of (a) Bloch-type, (b) Néel-type wall and (c) cross-tie wall

Anisotropy energy and magnetostatic energy terms. A variety of different domain wall configurations are possible by combining the basic Néel and Bloch type walls. These more complicated structures occur as the system tries to minimize the total energy. One common example is a cross-tie wall \([60, 61]\) (Figure. 2.6(c)) which, from Figure. 2.7, is found in film thicknesses of between 30\(\text{nm}\) and 90\(\text{nm}\) for Permalloy films.
2.3.2 Domain wall spin structures in nanowires

In a domain wall, the magnetization direction gradually change from one domain to the other. In soft magnetic structures like Py nanowires or nanostripes, the magnetization direction is restricted parallel to the wire axis because of the large shape anisotropy. Therefore, the spin structure of domain walls in these nanowires depends on the element width and thickness. Nakatani et al. [6] have established a refined phase diagram by numerical calculations and found different domain wall spin configurations which are energetically favorable for certain element widths and thicknesses. Figure 2.9 illustrates the wall types introduced by the phase diagram in Figure 2.8. These magnetic
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configurations are characterized by their axial magnetization alignment, which can be either head-to-head or tail-to-tail depending on if the magnetization are pointing towards or away from the wall, respectively. The vortex domain wall (Figure. 2.9(a,b)) consists of three distinct wall sections where the magnetization rotates about a central vortex core, an out of plane magnetization component. A vortex wall is also identified by the vortex chirality, which can be clockwise (Figure. 2.9(a)) or counter clockwise (Figure. 2.9(b)) depending on the sense of spin rotation about the vortex core. The transverse wall comprises, to a first approximation, two 90° walls with the spin in the central domain perpendicular (either magnetization pointing up or down) to the wire axis , (Figs. 2.9(c,d)). Besides these two basic types, an asymmetric transverse wall (Figs. 2.9(e-h)) is energetically favorable for certain element widths and thicknesses.

**2.3.3 Controlling of domain wall by geometrical features**

In order to control the position of domain walls in ferromagnetic nanowires various trapping sites such as notch and anti-notch of different geometries are used by fabricating along the nanowires [2, 6, 15]. To investigate the interaction of domain walls with notches and anti-notches a number of techniques including MOKE magnetometry [10, 16, 62], Lorentz transmission electron microscopy etc are employed [5, 11, 12, 18]. The strength of domain wall pinning by the geometrical pinning features along the nanowires was found to depend on the pinning geometry, wall types particularly the chirality of the incoming vortex domain walls [10, 62]. An exciting experiment was car-
ried out by K. J. O’Shea et. al. [63] on the controlled movement of DWs by fabricating anti-notch of variable width and height along the patterned Permalloy nanowires. The authors observed that the anti-notches present a complex potential landscape to domain walls. Moreover, the DWs can be trapped in front of, or be trapped inside the

anti-notches depending on the geometry of the latter and, in the case of vortex domain walls, the chirality. Figure 2.10 shows the same anti-notch acts either as a potential barrier or a well for the DWs. Figure 2.10 (a) demonstrates that upon the application of a magnetic field a CW VDW enters inside the anti-notch and therefore behave as a potential well. Figure 2.10 (c) shows that a cw VDW is pinned in front of an anti-notch of different height but same width. Therefore, in this case the pinning site acts as a potential barrier. Figure 2.10 (b) and (d) show schematically the corresponding local magnetization distribution of images 2.10 (a) and (c). A systematic study into domain wall pinning behavior as a function of geometrical confinement within planar nanowires was also carried out using MOKE magnetometry and OOMMF micromagnetic simulations [64]. It was observed clearly that the domain wall depinning field i.e the field to move the DW from the geometric structure increases as the wire width decreases, in particular for wires widths below 400 nm. Notably, for domain wall pinning at asymmetrical structures such as a notch, the magnitude of the depinning field appears relatively insensitive to notch geometry for triangular and rectangular notch structures, compared to the influence of the wire width. In Ref. [64], the authors observed the dependence of pinning behavior on wall chirality. The pining behavior
dependence upon wall chirality observed using MOKE magnetometry was in excellent agreement with that of micromagnetic simulations. In magnetic-field-driven nanowire devices, it is necessary to control the direction of DW motion to prevent walls from meeting and annihilating. The control of DW motion in one dimensional nanowire using geometrical features like symmetrical notch or anti-notch [Figure 2.11 (a)] along the nanowire axis allows DW propagation in one direction [16, 63, 65, 66]. These devices are analogous to electrical diodes since DWs moving in a “forward” direction depin from the element at a lower field than when moving in a “reverse” direction. A comprehensive investigation explored the underlying interactions governing DW depinning from symmetric and asymmetric diodes using micromagnetic simulations [4]. The results are shown in figure 2.11 and 2.12 Such a diode shaped anti-notch was considered in this investigation to investigate the influence of edge profiles of Permalloy nanowires.
on the controlled behavior of magnetic domain walls. This investigation was also carried out by using micromagnetic simulations although the edge profiles of Permalloy nanowires were modeled based on experimental investigations.

### 2.3.4 Energy profile of pinning sites

In order to provide a more quantitative understanding of the domain wall depinning behavior, the potential landscape for the DW states are calculated by micromagnetic simulations. The geometrical variations along the nanowire generate an energy landscape that a DW experiences while traversing through the wire. The change in the potential profile reflects the interaction between the spin structure of DW and the pinning site. In order to understand the energy landscape of the notch profiles, energy terms like magnetostatic and exchange energy are mainly taken into consideration. Usually a DW is initially placed on the left side, at a certain distance of away from the center of the notch. A constant magnetic field is applied along the +x-direction to drive the DW towards the right end of the nanowire, thereby, passing through the notches placed at the center of the nanowire. The absence of the anisotropy energy
term makes the energy equation converge to:

\[ E_{\text{Tot}} = E_{\text{mag}} + E_{\text{Ex}} \]  \hspace{1cm} (2.22)

where, \( E_{\text{mag}} \) is the magnetostatic energy and \( E_{\text{Ex}} \) is the exchange energy.

The total energy i.e. magnetostatic and exchange energy are carried out in this investigation and results are described in chapter 4.

In the next section, the best available technique (high resolution) for DW observation will be described.

\section*{2.4 Instrumentation & experimental techniques}

Microscopy is a technique used to capture visible images of structures too small to be seen by the human eye. The microscope itself has to accomplish three tasks: it must be able to produce a magnified image of the specimen, resolve features in the image and render the details visible to the eye or a camera. The technique has evolved with the development of optical technology and there are now three main branches: optical, electron and scanning probe microscopy. Among them the resolution of electron microscopy is much higher compared to that of others and therefore we have described here only electron microscopy for domain observation.

\subsection*{2.4.1 Electron microscopy}

The optical microscope is a familiar instrument for observing small objects using visible light. However, it is well-known that the resolution of a conventional optical microscope is limited by the wavelength of its illumination, so, the best optical microscopes in terms of resolution are only able to resolve features down to 380 nm [59]. Modern materials science and engineering requires a better microscope that can resolve features at a smaller length scale down to the atomic scale. In 1925, Louis de Broglie [67] hypothesised that electrons exhibit wave-like characteristics, with the possibility of
wavelengths far shorter than visible light:

\[
\lambda = \frac{\hbar}{p}
\] (2.23)

with \( \hbar = 6.625 \times 10^{-34} J.s \) is the Planck’s constant, and \( p \) is the momentum of the particle. This leads to the idea of designing a microscope using the electron wave to overcome the resolution limitation of conventional optical microscopes. With an electron moving through an accelerated voltage of 100\( kV \), the wavelength is about 3.70\( pm \) (3.70 \( \times 10^{-12} \) \( m \)), which is much shorter than that of the visible light. It means that if electron waves can be used in imaging technologies and therefore a superior resolution is possible to obtain.

Convensional transmission electron microscope (CTEM)

The first electron microscope (transmission) was built in 1933 by German physicists Ernst Ruska and Max Knoll and was similar in design to the optical microscope. Using electromagnetic lenses to focus a beam of electrons, this instrument was capable of magnifying objects 400 times. Electron microscopes have come a long way since this model, with modern versions being able to resolve individual columns of atoms in crystals with magnifications of several million times [68]. The original form of electron microscopy, transmission electron microscopy [69], involves a high voltage electron beam emitted by a triode electron gun and focused by electromagnetic lenses. The beam is partially transmitted through a very thin specimen, carrying information about its physical structure.

2.4.2 Scanning transmission electron microscopy (STEM)

The scanning transmission electron microscope [70] is a hybrid of the TEM and SEM which uses deflection coils to scan a fine electron probe across the surface of a thin specimen, and is generally used to localize signals at very high resolution. Often the deflection coils are built into modern TEM systems to enable STEM imaging in addition to the usual TEM modes of microscopy, but dedicated STEMs are also available.
2.4.3 Lorentz Microscopy

In order to observe directly the magnetic domain and domain walls in ferromagnetic materials a special branch of TEM named as Lorentz TEM is used [71]. Magnetic imaging using Lorentz TEM [72, 73] rely on small deflections of electrons on passing through thin magnetic specimens. These deflections are a consequence of the Lorentz force and are used to generate contrast in a magnetic sample [12]. When electrons are incident on a thin magnetic specimen, the interaction of electrons with the specimen can be described by both classical and quantum mechanical approaches by considering electrons as particles and waves, respectively.

In Lorentz microscopy, if the electrons are considered as particles, magnetic contrast is generated by the deflection of electrons on passing through a magnetic specimen with a component of induction perpendicular to the electron trajectory. Electrons traveling along the z-axis through a magnetic sample with an in-plane magnetization, will experience deflection in the x-direction as a result of the Lorentz force, \( F_L \) given by,

\[
F_L = -e(E + v \times B) \tag{2.24}
\]

B is the magnetic induction in the specimen, e, v are the electron charge and velocity.

![Figure 2.13: Schematic illustration of the principle of Fresnel imaging mode. The main imaging lens is defocused a distance above or below the specimen plane to observe contrast at the positions of domain walls and at the edges of the elements.](image)

The above classical description by considering electrons as particles is sufficient to qualitatively explain the principles of Lorentz microscopy. However, to extract quan-
quantitative magnetic information, a quantum mechanical approach using the Aharonov-Bohm effect [74] is essential.

For in situ investigation of magnetization reversal behavior in ferromagnetic nanowires, the Fresnel mode of Lorentz TEM is a powerful technique. Schematic diagram illustrates that electrons passing through an in-plane magnetized film are deflected in opposite direction by the neighboring 180° anti-parallel magnetic domains. Magnetic domain walls become visible in a defocused image as alternating black and white lines due to alternating convergence and divergence of the electron beam at the wall position, whilst the domains themselves appear with near-uniform electron intensity. Figure 2.10(a and c) are the examples of Fresnel images which show DWs as black and white lines.
Chapter 3

Micromagnetics Simulation

Previous chapter provides insight about basic ferromagnetism, in particular domain wall spin structure in ferromagnetic elements. This chapter will discuss details about Micromagnetic study using Computer simulations. To study magnetic behavior in a ferromagnetic element either analytical models or practical experiments to be used. Analytical models exist only for few magnetic systems, however for these models solutions are only practical for simple cases. Experiments allow observations to be made of real systems, but we are limited to the detail which can be extracted from these measurements. When computational resources are available, more complicated models can be used which provides a link between experiment and theory. The motivation for using computer simulations is two-fold: firstly, it is possible to interpret experimental results, and secondly new design can be predicted, subsequently developed and definitely these are cost effective.

3.1 Computational Micromagnetism

Two software packages are available to perform simulations in computational micromagnetics. First, the Object Oriented Micromagnetic Framework OOMMF [19] developed by the National Institute of Standards and Technology. OOMMF employs the finite difference (FD) method which requires the discretization (or segmentation, please see section 3.2) of a chosen geometry over a grid of cells each of identical volume and cuboidal shape. The second is magpar [75, 76], developed by Werner Scholz and
the group of Prof. Fidler and Prof. Schrefl of the Technische Universität Wien. This software uses the hybrid finite element (FE)/boundary element (BE) method which requires tetrahedral volume geometry as discretized volume elements. The volume elements can be of variable volume and shape.

Among these two techniques, OOMMF is being used widely to understand the behavior of the magnetic domain walls in ferromagnetic nanowires. An excellent qualitative agreement was observed between experimental observation and outcome of OOMMF simulation in a number of investigations (Refs. [7–10] are examples of few). For this present investigation the freely available OOMMF code was used. The OOMMF code calculates micro-magnetism by solving Landau-Lifshitz-Gilbert equation. Notably, micromagnetic simulations based on Landau-Lifshitz and Landau-Lifshitz-Gilbert equations of motion has become an important tool to characterize the magnetic behavior of different materials like recording media, patterned magnetic elements and nanocrystalline permanent magnets. The Landau-Lifshitz-Gilbert equation will be described in the following section.

### 3.1.1 Object Oriented Micromagnetic Framework (OOMMF) and Landau-Lifshitz-Gilbert equation (LLG)

To determine the magnetization distribution that minimizes the total energy of the system, Landau-Lifshitz (LL) equation of motion is given by,

\[
\frac{d\mathbf{M}}{dt} = -|\vec{\gamma}|\mathbf{M} \times \mathbf{H}_{\text{eff}} - |\vec{\gamma}|\alpha \frac{M_s}{M_s} \mathbf{M} \times (\mathbf{M} \times \mathbf{H}_{\text{eff}}) \quad (3.1)
\]

where, \(\mathbf{M}\) is the magnetization (i.e. the magnetic moment per unit volume), \(\mathbf{H}_{\text{eff}}\) is the effective magnetic field, \(\alpha\) is the Landau and Lifshitz phenomenological damping parameter and \(\vec{\gamma}\) is the Landau and Lifshitz electron gyro-magnetic ratio (the ratio of the magnetic dipole moment to the mechanical angular momentum of some system). If one assumes,

\[
\gamma = (1 + \alpha^2)\vec{\gamma} \quad (3.2)
\]
then this can be shown to be mathematically equivalent to the Gilbert form [77]:

$$\frac{dM}{dt} = -|\gamma|M \times H_{eff} + \frac{\alpha}{M_s}(M \times \frac{dM}{dt}) \quad (3.3)$$

Now, the time independence of the magnetization can be obtained directly from the quantum mechanical expression for the precision of magnetization in a magnetic field,

$$\frac{dM}{dt} = -\gamma M \times H_{eff} \quad (3.4)$$

Where \( t \) is the time, \( \gamma \) is the gyro-magnetic ratio and \( H_{eff} \) is an effective field,

$$H_{eff} = -\frac{1}{\mu_0} \frac{dE_{tot}}{dM} \quad (3.5)$$

which takes into account the exchange, anisotropy, magnetostatic and external field interactions where \( E_{tot} \) is the total energy of the system. The micromagnetic simulation program evaluates the effective field at each cell in the uniform discretized grid of the problem domain and the resulting magnetization by solving the Landau-Lifshitz (LL) equation,

$$\frac{dM}{dt} = -\gamma M \times H_{eff} - \frac{\lambda}{M_s^2}M \times (M \times H_{eff}) \quad (3.6)$$

Where \( \lambda \) is a damping parameter, \( H_{eff} \) is the effective field and \( M_s \) is the saturation magnetization. Gilbert proposed a different damping term however to overcome the limitations in the LL equation for ferromagnetic materials with large internal damping to give the Landau-Lifschitz-Gilbert equation (LLG),

$$\frac{dM}{dt} = -\gamma^* M \times H_{eff} + \frac{\alpha}{M_s}M \times \frac{dM}{dt} \quad (3.7)$$

with damping coefficient, \( \alpha \). The two equations, 3.6 and 3.7, are equivalent provided the \( \gamma^* = \gamma(1 + \alpha^2) \) and \( \alpha = \lambda/\gamma M_s \). The first term in the equation describes the precision of the magnetization vector \( M \) around the effective field, \( H_{eff} \). The second term describes the dissipation of energy and describes the motion of the magnetization towards the effective field, \( H_{eff} \), as illustrated in figure 3.1. With each spin iteration,
the equation is re-evaluated until equilibrium is reached. Equilibrium may be defined by a minimum value of the torque, $dM/dt$, typically set to $1 \times 10^{-5}$, or by a limit on the number of iterations or simulation time. This process is repeated with each step-wise increase of the applied field. An ideal simulation of a nanomagnet would include every atom in the system, however this is not achievable due to constraints of available computing power and time. Instead the nanomagnet or nanowire in our investigation may be divided up into a set of discrete 3-dimensional cells of uniform magnetization as described in the next (section 3.2). The cell size is an important parameter in determining the outcome of the simulation and is user defined. Typically a cell size close to the exchange length provides realistic results whilst keeping the simulation time to a manageable length. The simulations performed in the thesis used a cell size of 5 nm which is close to the exchange length for Permalloy ($Ni_{80}Fe_{20}$).

### 3.2 Discretization of the simulation sample

When a particular geometry is decided for simulation, this must be discretized into lots of smaller cuboidal cells to be able to use the finite difference method. Each cell is considered to be homogeneously magnetized, i.e. within a micromagnetics simulation all of the atomic magnetic moments inside this cellular domain are thought to behave as a single particle. This is an acceptable assumption because at an atomic length scale the exchange interaction, responsible for the homogeneous alignment of magnetic moments, is overwhelmingly one of the most significant energy term. The separate
simulation cells represent a certain amount of magnetic material. Obviously in this instance a finer discretisation mesh, a smaller simulation cell size, is more desirable than a coarser mesh, particularly when there are curved surfaces in the geometry.

OOMMF use finite difference method (FDM) to solve Landau-Lifshitz-Gilbert equation for detail please see chapter 3 section 3.1. Yet another more modern technique widely used is Finite Element Method (FEM), which is more concern with the integral form of the differential equation. FDM uses small three dimensional cube like spatial distribution to define the shape of the object under consideration, the primary drawback is the limitation of defining irregular object geometry with high accuracy, whereas with FEM a triangular mesh like structure can be used to define the geometry of the object which is more easier and accurately represent the sample. Figure 3.2 demonstrates the effect of altering the number of cells in a geometry. In the case of extremely coarse discretisation using the finite difference method, a sphere can resemble more a cuboid than a sphere (figure 3.2, left). A poor representation of the shape in the discrete model can affect the influence of the shape anisotropy (please see section 2.2.2) on the magnetization, and subsequently negatively affect the results. Figure 3.3 shows the discretisation of a shape using both fixed size cubic cells (finite difference) and variable sized tetrahedral cells (finite element). In this sphere example, there are four times fewer cells in the finite element example yet it is aesthetically more sphere-like.

The exchange length is a length scale over which the direction of $\mathbf{M}$ does not change significantly. A coarse mesh will not allow the software to resolve the exchange length properly, so independent domains will not form correctly. The exchange length is
calculated by considering [78, 79]:

\[ \lambda_{ex} = \sqrt{\frac{A}{2\mu_0 M_s^2}} \]  

(3.8)

where \( A \) is the exchange energy (measured in \( J/m \)), \( \mu_0 \) is the magnetic constant \( (4\pi10^{-7}T.m.A^{-1}) \) and \( M_s \) is the magnetization in \( A/m \). The exchange length \( \lambda_{ex} \) therefore gives us a quantitative measure for the required mesh resolution. The derivation of the exchange energy in the micromagnetic theory uses the Taylor series expansion of the cosine between two moments to the second-order:

\[ \cos \phi_{ij} \approx 1 - \frac{\phi^2_{ij}}{2} \]  

(3.9)

It is crucial that the maximum angle between these two adjacent moments is not high [80] - indeed if the angle becomes larger than \( \pi/2 \) radians, then the results of the simulation are highly inaccurate as the torque between the two spins begins to decrease when the angle is further increased; this could potentially lead to the scenario where the angle between two adjacent spins is \( \pi \) radians - according to the second-order Taylor expansion of the cosine, this would be a perfectly legitimate low-energy state, although this is clearly not the case as the exchange energy and consequently the torque between these two spins in this state would be extremely large. Incidentally,

**Figure 3.3**: Finite difference (left) and finite element (right) meshes. For adequate shape resolution the finite difference model requires more cells than the finite element model; in this case 27000 and 5000 respectively

it is worth noting that since the simulation is not atomistic, the use of the discretized version of the micromagnetic expression for the exchange energy 3.8 is always slightly inaccurate from a quantitative perspective, however if the angle between two spins is
greater then $\pi/2$ radians then the behavior becomes qualitatively wrong. The answer to these problems is of course to create a finer mesh; however if one makes the mesh $n$ times as fine, then the number of cells in the simulation increase by $n^3$ (since the system is three-dimensional) and this results in a massively increased computational overhead. Moreover, in case of the triangular mesh it is particularly difficult to maintain the exchange length within which there is no magnetic interactions. So, in order to reduce the computation time of the simulation we have used a cube of 5 nm length, which is our exchange length for Permalloy, to graphically design the input file so that a balanced condition between finer mesh size and number of cell to represent the total sample can be achieved.

### 3.3 Material parameters used for simulations

In this investigations, we intent to study the influence of the edge profile of Permalloy nanowires on the magnetic behavior of domain walls using micromagnetic simulations. Therefore understanding of the material parameters of Permalloy is extremely important. The standard parameters for Py are saturation magnetization $M_s = 8.6 \times 10^6 A/m$, exchange stiffness constant $A = 1.3 \times 10^{-11} J/m$, magnetocrystalline anisotropy $K = 0$ and damping coefficient $\alpha = 0.5$ [81–83]. The measured damping parameter $\alpha$ for Py estimates between 0.013 and 0.03. However, a damping parameter of 0.5 was used throughout to speed up the computations as was mentioned earlier. A cell size of $5 \times 5 \times 2nm^3$ was used. The cell size in x-direction and y-direction is chosen to be equal to the exchange length for Permalloy whereas to simulate the edge profile of the nanowire reasonably we chose $2nm$ cell size in z-direction. The continuous geometry of the actual nanowire edge will be represented discreetly as boxes in 3-dimension by the OOMMF simulation software. So, to achieve more closer to the actual edge profile a much smaller cell size is chosen for the z-direction. As the applied magnetic field is acting in the x-direction which restrict the domain rotation only in xy plane choosing a smaller length than exchange length in z-direction would not compromise the calculation precision.
3.4 Experimentally observed edge profiles of Permalloy nanowires

Miniaturization, i.e. all the way down to the atomic scales, with improved performance is the main theme of modern nanofabrication technology. The advancement in nanofabrication technology opens fascinating opportunities for engineering innovative magnetic materials and stimulates the demand for magnetic storage devices with higher density, faster speed, lower power consumption and smaller size than the current state-of-the-art devices. Among a variety of nanofabrication techniques, electron beam lithography (EBL) is widely used since the late 60s for high resolution sub-micron scale patterning of micro/nanostructures. The processing steps of the EBL technique are shown schematically in figure 3.4(a). Electrons can effectively expose any materials

![Figure 3.4: Schematic illustration of the processing steps of two alternative lithographic techniques. The processing steps for writing patterns using (a) EBL technique and (b) FIB milling technique. The latter technique is faster and a new addition to the range of nanofabrication techniques.](image)

but due to their very light mass exposing of the electrons change properties of soft materials, such as photo-resist or electron beam resist. The principal component of a resist is a high molecular-weight polymer dissolved in a liquid solvent. The polymer changes its structure when exposed to radiation, including electron radiation. Electron beam resist can be classified as either negative or positive resist. After exposure to electrons, the positive resist is weakened by chain scission to produce organic molecules

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of a lower molecular weight. These lower molecular weight resists wash away by the solvent developer and eventually a positive tone pattern is formed in the resist film, figure 3.5(a). On the other hand, the negative resist is strengthened during exposure by random cross-linkage of main and side polymer chains and become less soluble in the developer, figure 3.5(b). Therefore, with negative resist, the unexposed resist portion is removed during the developing process. On the contrary, with positive resists only the unexposed portions remain after developing, as was explained earlier. Most commonly used positive resist Poly-methyl Methacrylate (PMMA) was used by M. A. Basith et. al. [9] for patterning nanowires in the present investigation and the size of the electron probe in conjunction with resist determined the resolution of the pattern generation. The resist thickness depends on the PMMA concentration and spinning speed. Single layer PMMA often causes improper lift-off, figure 3.6(a). A bilayer PMMA resist was used for lift-off process, figure 3.6(b). To accomplish the lift-off process, after metallization the substrate is immersed in a solvent that dissolves the resist but does not attack the metal film. This step ensures that the polymer and any overlying metal as removed and the metal is only present in the regions specified by the pattern. However, in practice, a build up of metal on top of the PMMA resist was observed in the cross-sectional TEM images of the EBL patterned nanowires described later on. An alternative approach, however, for writing patterns on thin continuous
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Figure 3.6: Schematic illustration of the resist and deposited metal profile with (a) a single resist layer and (b) a bilayer of electron sensitive resist. The later one facilitates the subsequent lift-off process of the resist, forming a suitable undercut profile.

Figure 3.7: TEM bright field image of edge profile of the nanowire showing different layers films may be the focused ion beam (FIB) milling technique. This technique is a new addition to the range of nanofabrication techniques and is comparatively faster than other current micro/nanofabrication techniques for the fabrication of prototype micro/nanostructures [11, 84–88]. The processing steps of the focused ion beam milling technique are illustrated schematically in Figure 3.4(b).

Cross-sectional samples were prepared using FIB milling to observe the details of the nature of the physical structure of the patterned nanowires around their edges [9, 87]. Transmission electron microscopy (TEM) experiments like bright field cross-sectional TEM imaging were performed to compare the nanostructures produced by these two technique namely electron beam lithography and focused ion beam milling. Figure 3.7 shows cross-sectional TEM bright field image of a nanowire patterned by EBL technique. The individual layers were also labeled in this Figure 3.7. The high magnification cross-sectional TEM images demonstrates the left edge structure of the
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EBL (Figure 3.8B and FIB patterned (Figure 3.8A) nanowires.

As another example, similar edge profiles are not only observed in Permalloy nanowire but also in array of Permalloy nanodots. A lorentz TEM characterization study on physical structure of nanostructure magnetic thin films [89] demonstrate the sloped and tapered edge profile formation in specimen series fabricated by EBL technique.
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Figure 3.9A shows a 45° sloped edge profile, whereas 3.9B demonstrates the formation of a 60° sloped i.e., tapered edge profile. The Permalloy thickness of the specimen is 20 nm.

Based on the experimentally observed edge profiles we proposed nanowire with sloped and tapered edge profile to further study of the influence of edge profile on magnetic behavior or domain wall using micromagenetic simulations. Modeling of the nanowires are described in the following section (section 3.5).

A comparison of the edge structure from the cross-sectional images of the EBL and FIB samples indicate that in both cases the edge profile is not vertical but tapered, though in the case of the FIB structure the tapering is slightly less symmetric [9]. Whilst in the case of the EBL nanowires the tapering may be in part due to residual resist, in the case of the FIB nanowires this is clearly due to the interaction of the
Ga+ beam with the film during the milling process. However in both cases the edge structure can be described as well defined. A recent investigation also demonstrates the tapered edge profiles of Co nanowires [Figure 3.10] fabricated by FIB irradiation [14].

3.5 Modeling of the edge profiles of the nanowires

The described experimental investigations clearly demonstrated that the edge profiles of the patterned nanowires are either tapered or nearly sloped and varied slightly from wire to wire. Notably, a rectangular cross-section (vertical) of the wire edge is generally considered to conduct micromagnetic simulations which is ideal rather than real. Therefore, in the present investigation we have modeled three different edge profiles of Permalloy nanowires and investigated the propagation of DWs along these nanowires along with their interaction with geometrical anti-notch. The edge profiles of Permalloy nanowires considered for this investigation are shown as schematic cross-section of the wires in figure 3.11 in which 3.11A was designed as an ideal structure with a rectangular cross-section and figure 3.11B was structured based on the TEM cross-sectional image of figure 3.8A and 3.9A, whereas, the edge structure figure 3.11C was modeled based on the TEM cross-sectional image figure 3.8B and 3.9B. The width of the nanowires has been reduced for this schematic indicated by vertical cuts.

The nanowires with rectangular, sloped and tapered edge profile were referred as model 1, model 2 and model 3, respectively throughout the investigation. The edge profiles was modeled by dividing the nanowire in 5 layer each of 1 cell (2nm) height. By keeping the wire width at layer 1 and reducing each layer width by 2 cells (10nm) gradually from layer 2 to layer 5 the sloped edge profile was modeled. Similarly tapered edge profile was modeled by keeping layer 3 same as the wire width and reducing layers 2,4 and layers 1,5 gradually by 2 cells (10nm), figure 3.11.

Micromagnetic simulations were performed for transverse up(TUP), clockwise (CW) and counter-clockwise (CCW) vortex domain wall (VDW) configuration, figure 3.11. Figure 3.12 (a,b) illustrate schematically the plan view of nanowires with symmetric and asymmetric anti-notches, respectively. For modeling TUP DW the width of the
Figure 3.11: Schematic of the nanowires with standard rectangular, sloped and tapered edge profiles. The sloped edge was modeled based on experimental images showed in figure 3.8A and tapered edge based on images showed in figure 3.8B respectively. The nanowires with rectangular, sloped and tapered edge profiles were referred as model 1, model 2 and model 3, respectively. The vertical cuts illustrate the reduced wire width in these schematics.

The wire was varied from 100 nm to 180 nm for fixed 10 nm Py thickness. On the other hand, for modeling VDW (CW/CCW) the wire width was varied from 180 nm - 300 nm for the same Py thickness. There were chosen based on DW structure phase diagram [6]. A diode shape anti-notch of 100nm height and 150nm width with both symmetric and anti-symmetric nature is used as a pinning site for magnetic domain wall as shown in figure 3.12 with the height and width of the anti-notch. The idea behind choosing a
Figure 3.12: Schematics of the nanowire geometries with symmetric and asymmetric anti-notches are shown in figure 3.12A and 3.12B, respectively.

The diode shaped anti-notch has been discussed in detail by M. T. Bryan et al. [4] which shows the domain wall controlling with symmetric and asymmetric anti-notch. A diode shaped anti-notch provides the ability to control precisely particular type of domain wall as well as they are easy to fabricate.

3.6 Computational issues

To perform micromagnetic simulations, two different procedures are necessary depending on whether the OOMMF software [19] is used to determine the demagnetizing field.

Figure 3.13: The simplified simulation process. The left-hand side of the chart represents the input files for the simulation packages for OOMMF (finite difference method; the micromagnetic information format file contains material, simulation and geometric parameters) or magpar (hybrid finite element/boundary element method, material; simulation and geometric (mesh) parameters as individual files). The results from each of these packages are transformed into unified output formats (right-hand side) for analysis (xmgrace [90]) and visualization toolkit (VTK).

3.6.1 OOMMF software requirements

We use three pieces of software to perform micromagnetic studies with the finite difference method. Each of these packages is an extension on other widely available
applications (see figure A.1 and Appendix A).

The first piece of software is a proprietary program, mifmaker, which we developed to create simulation environments. In general a significant amount of manual effort is required to generate a simulation, as the problem must be directly defined in a Tcl-based format which OOMMF can recognize. There is no method built-in to OOMMF which allows this process to be automated for three-dimensional problems. The mifmaker program is a command-line application which can accept a series of geometric, material and simulation parameters and generate a valid description to solve the problem.

On the other hand mif file can be produced manually using any text editor by precisely following a standard template for mif files. This investigation has done by this as we use the remote Linux cluster provided by Cluster Authority of Rajshahi University for faster calculations which doesn’t has a GUI support. mif files entry must be very precise, even an extra space or character or punctuation can break the script while compiling.

Upon generating the required files, this is sent to OOMMF — the Object Oriented Micro-magnetic Framework — developed by the National Institute of Standards and Technology. OOMMF can then solve the micromagnetic problems presented by the mif/mif2 file. OOMMF is highly dependent on Tcl/Tk [91–95]. Figure 3.14 shows how the requirements for system memory in OOMMF scale in a cubic system (i.e. the length of the $x$, $y$ and $z$ sides of the cube are the same length and have the same discrete cell size) as a function of the number of cells.

\section*{3.6.2 Hardware requirements}

Theoretically, physical simulation software have modest hardware requirements, however as with all simulation problems of this nature “bigger is better”. Ideally, a machine with a minimum of one gigabyte of RAM should be used to maximize the size of the potential problem which can be solved.

Each discrete cell within a micromagnetic problem to be solved with OOMMF consumes approximately one kilobyte of RAM, therefore to solve a system with $1 \times 10^6$
Figure 3.14: The memory requirements of OOMMF as a function of the number of discrete simulation cells per edge for a three-dimensional geometry.

cells, one gigabyte of RAM is required just to run the simulation. This is without taking into account the size of the simulation package itself, which must be loaded into RAM and creates a fixed overhead.

Once operating system overheads are considered, it is clear that the amount of physical system RAM available to a machine should be greater than the amount of RAM required by the simulation — this is primarily to avoid “thrashing”, a situation where the operating system is forced to temporarily write (“swap”) areas of the RAM to the hard disk and read other areas back into RAM from the disk. The precise amount of RAM required for operating overheads will vary from system to system; a system dedicated and optimized for performing only simulations may only need a few megabytes reserved for the operating environment, but a workstation which is running other applications concurrently e.g. visualization software, e-mail clients, document editors and Internet web browsers) may require several hundreds of megabytes.

Notably the access times in modern hard disks are several orders of magnitude greater than those of RAM (these access times are measured in milliseconds for hard disk drives and nanoseconds for RAM), this will slow down any particular simulation by this factor, making successful completion of the simulation impossible from a practical standpoint. Even in an optimized scenario where data seek latency is eliminated, the
hard disk can be expected to deliver data approximately 100 times more slowly than RAM [96].

The speed at which the processor can perform floating point calculations is overwhelmingly the primary factor when considering the time a simulation will take to complete. Any processor which has a fast floating point unit coupled with a compiler which is able to take maximum advantage of this floating point unit when optimizing the simulation source code is ideal — through our own studies we note that carefully chosen compiler options can increase the execution speed of the simulation three fold.

Additional methods such as high-throughput batch processing [97, 98] and clustering allow either sets of simulations to be performed (e.g. many small computations such as those needed for phase diagrams) or larger computations which would be impossible to compute with neither the memory capacity nor the processing power of a supercomputer. OOMMF, unlike magpar, is unable to take advantage of the message-passing interface [99, 100] common to computational clusters.

### 3.6.3 Disk space requirement

A collection of large hard disks is also beneficial to allow the long-term storage of simulations previously completed, assisting with the rapid retrieval of past vector data created by simulations.

Either 32-bit (single precision) or 64-bit (double precision) floating point numbers can be used to store the components of the vector data. The case for selecting one precision over another can be argued from two perspectives: storing 32-bit numbers will save disk space if the extra precision offered by 64-bit numbers is not necessary, however vector interpolation used by certain visualization techniques (e.g. the calculation of streamlines) may benefit from a higher-precision. It is worth noting that OOMMF performs the simulation using double precision numbers irrespective of the precision of the output format.

Double precision floating point numbers usually require eight bytes of storage each. To store the magnetization vectors for a given mesh in OOMMF, each position of the mesh requires three 64-bit numbers to describe it \((\mathbf{x}, \mathbf{y} \text{ and } \mathbf{z} \text{ components})\). This
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gives a simple equation for calculating the amount of space needed to store one set of magnetization data for a simulation:

\[ s = \alpha + \frac{l_x \ l_y \ l_z \ 3p}{c_x \ c_y \ c_z \ 8} \]  

(3.10)

where \( \alpha \) is the space consumed by a header describing the relationship between the vector data and the simulation, \( l_x, l_y \) and \( l_z \) represent the size of the complete mesh, \( c_x, c_y \) and \( c_z \) are the edge lengths of the discrete cell and \( p \) is the number of bits used to store one floating point number. Note that with OOMMF, even empty cells (i.e. where \( |M| = 0 \)) are stored by default.

For example, to store the magnetization vectors for a sphere of diameter 120nm \((l_x = l_y = l_z = 120 \times 10^{-9}m)\) with a cubic mesh cell size of 5nm\(^3\) \((c_x = c_y = c_z = 5 \times 10^{-9}m)\) with 64-bit precision \((p = 64)\), \((120/5)^3(83) = 331776\) bytes of disk space are needed, plus a small fixed overhead. If a coarser mesh were used, such that \( c_x = c_y = c_z = 10 \times 10^{-9}m \), then only 41472\( bytes \) of disk space are necessary to store the magnetization data for one time-step.

For a complete simulation many sets of magnetization vector data are stored, each usually representing a particular "stage" - a point where the magnetization configuration for an externally adjustable factor, such as applied magnetic field, is considered stable. A typical simulation might have 100 of these stages. In the case of the sphere example above, this equates to over 31\( megabytes \) of disk space. For a sphere of double the diameter with a high field step resolution (giving 1000 stages if \(-500mT \leq B_x \leq 500mT \) and \( B_x \) is reduced in 1mT steps), over 2.5\( gigabytes \) of storage space would be necessary. Doubling the mesh resolution and the diameter further, such that \( c_x = c_y = c_z = 2.5nm \) and \( d = 480nm \), the amount of required disk space grows to well over 150\( gigabytes \).

### 3.6.4 Post-processing

Finally, to visualize the results of our simulation, the magnetization vector data-sets are transformed from the OOMMF format to the Visualization Toolkit (VTK) format, an open standard for visualization. These results are visualized with MayaVi, a piece
of data visualization software initially developed to assist with the visualization of computational fluid dynamics environments. Finally the visualization files, with avf extension, are converted in to standard image files using avf2ppm script provided with OOMMF software package. This script file avf2ppm can be taken various settings to produce desired output design, \textit{i.e.} magnetization direction arrow, arrow size, color region for each magnetization direction etc.

All of these applications should run in any operating system environment for which an ANSI-compliant C/C++ compiler is available, however in this project we have only made extensive use of GNU/Linux and Microsoft Windows machines running on either Intel or AMD processors.

We have written many other smaller scripts to assist with pre-processing and post-processing of data files generated by all of the aforementioned applications.

### 3.6.5 Simulation Procedure

First step of running micromagnetic simulation is to model the nanowire by designing an image file of ppm extension. The image file shows different magnetic regions by different color. Magnetically neutral part of the image is also designated by a distinct color. Second step is to create an input file of mif/mif2 format that contains all the required parameters including the magnetic domain defined by colored region, their dimension, magnetization direction, all other parameters required like the values of $M_s$, $A$, $K$, $\alpha$ etc. Input files also holds information of output files and location of all the required input files and output directory, number of steps of the simulation for calculations, cell size of magnetic domains for discretization of the nanowire.

Once all the necessary files are prepared, simulation can be run on interactive mode using the graphical user interface (GUI) of the OOMMF software if available. OOMMF can also be run from command line interface (CLI) using appropriate commands. In this investigation we use the CLI to run the simulation.

The results of this investigation are discussed in chapter 4.
Chapter 4

Results and Discussion

Previous chapter, chapter 3, described the computational micromagnetism in detail along with the discretisation of the elements to be simulated. It also covered the modeling of the structure of the wire edge based on experimentally observed edge profiles of the fabricated nanowires. In this chapter we will present the results on the magnetic behavior of DWs along the nanowires of different edge profiles by using simulation package OOMMF.

Micromagnetic simulations are among the most widely used tools to understand the dynamic behavior of the domain wall under applied magnetic field. In this investigation the simulation package Object Oriented Micromagnetic Framework (OOMMF) is used to simulate nanowires with different edge profiles. Since many years, a rectangular cross-section of the edge profile of a nanowire is modeled for micromagnetic simulations [4, 101–103], whereas, in actual practice, using advanced nanofabrication technique a perfect rectangular cross-section of the nanowire edge is highly unlikely rather the edge of a fabricated nanowire is always sloped or tapered [9, 14]. In this investigation we have considered these two experimentally observed edge profiles of the nanowires to explore their influence on the controlled motion of DW along the nanowire. In this investigation we have simulate nanowire with width from 100 nm to 180 nm for transverse domain wall and 150 nm to 300 nm for vortex domain wall configuration [6] with diode shaped anti-notch [4] as a pinning site. To find out the effect of chilarity on the pinning of DWs both symmetric and asymmetric anti-notch were modeled. All these nanowire width was considered for three models of edge profile, rectangular referred as model 1, sloped
referred as model 2 and tapered referred as model 3. Nanowires were 3000 nm long and have had a Permalloy thickness of 10 nm. The precise control of a domain wall in a Permalloy nanowire depends on various factors. In this investigation the influence of the edge profile on major aspects like the total energy and the ground state energy landscape of the nanowires, energy prior to depin of the domain walls, depinning field i.e. the field required to escape the DW from the anti-notch, and the chilarity effect are observed and discussed in details in the following sections.

4.1 Energy Landscape

For a better understanding of the domain wall behavior, the energy landscape for the DW states is calculated by micromagnetic simulations [64, 104]. The energy landscape is generated by the geometrical variations along the nanowire that a DW experiences while traversing through the wire. The change in energy profile shows the interaction between the spin structure of DW and the pinning site [64]. In order to understand the energy landscape of the nanowire with diode shaped anti-notch, energy terms like magnetostatic energy and exchange energy are taken into account. A DW is initially modeled on the left side, at some distance from the center of the anti-notch. Then the modeled nanowire was relaxed by running the simulation with 0 (zero) applied magnetic field during which the domain inside the nanowires are orient in order. After relaxation, a constant magnetic field is applied along the positive x-direction to drive the DW towards the right end of the nanowire through the anti-notch. The absence of the anisotropy energy term makes the energy equation converge to,

\[ E_{Tot} = E_{mag} + E_{Ex} \]  \hspace{1cm} (4.1)

where, \( E_{mag} \) is the magnetostatic energy and \( E_{Ex} \) is the exchange energy [105]. Thus the total energy landscape give us a complete picture of the energy profile of the nanowire at various domain wall positions, i.e. in relaxed state, in state prior to depinning of the domain wall. Energy profiles for transverse up and vortex domain wall configurations are described in the followings sections 4.1.1 and 4.1.2.
4.1.1 Energy profile of a transverse up domain wall

As was mentioned in Chapters 1 and 2, the transverse wall comprises as a triangular, transversely oriented domain bounded on two sides by a ”V” configuration of 90° Néel walls oriented diagonally to the strip axis [106]. It has reflection symmetry about a line perpendicular to the strip axis, and a lack of symmetry about the center line of the strip. Figure 4.1 (a) shows the schematic diagram of a planar nanowire along with a transverse DW at the left side of the wire and an asymmetric anti-notch at the middle of the wire. The corresponding magnetization distribution of the head to head transverse up (TUP) domain wall is shown in the simulated image, figure 4.1(b). Notably, throughout the simulations, the Permalloy thickness is 10 nm, the width and height of the anti-notch are 150 nm and 100 nm respectively. These values are fixed and only the width of the nanowires was varied. Figure 4.2 (A) demonstrates the total energy as a function of normalized magnetization for 160 nm wide nanowire with symmetric anti-notch for rectangular (model 1), sloped (model 2) and tapered (model 3) edge profiles. The wall structure here is TUP and this is a representative wire width for all other transverse walls modeled here according to DW structure phase diagram [6]. The significant energy points inside these curves were marked by points a to e for model 1 and f to j for model 2. The corresponding simulated images shown in figure 4.2A (B) illustrating the pinning behavior of TUP domain wall, images (a) to (e) for nanowires with rectangular (model 1) edge profile and images (f) to (j) for sloped (model 2) edge.
Notably, these images are corresponding to the marked points in graph 4.2A. The total energy as a function of normalized magnetization does not differ significantly between nanowires with sloped (model 2) and tapered (model 3) edge profiles and therefore, throughout the investigation the energy values of nanowires with sloped edge profiles were described in details and compared with nanowires having ideal rectangular edge profile. The energy diagram, figure 4.2A, clearly demonstrates that total energy of nanowire with rectangular edge profile is significantly higher than that of nanowires having sloped and tapered edge profile. The energy point ‘a’ in figure 4.2A is ground state energy and by the application of a magnetic field of up to 30 Oe, the TUP DW doesn’t move anymore from the corner position of the nanowire and the energy value remain unchanged. Upon the application of a magnetic field of 40 Oe the domain wall trapped inside the anti-notch, simulated image (b) of figure 4.2B and in this state energy values fall down and this is correspond to point ‘b’ in the energy diagram. For a further increment of the applied magnetic field up to 110 Oe (simulated image c), the DW remain trapped inside the anti-notch and energy values doesn’t change significantly. The wall structure was found to extend over a large distance from the anti-notch of nanowire having rectangular edge profile for an applied magnetic field of 130 Oe. This state corresponds to simulated image (d) and energy point ‘d’ in the energy diagram 4.2A. Due to the large extension of the wall structure, at this stage the energy, mainly, magnetostatic energy was increased significantly. An applied magnetic field of 140 Oe depinned the domain wall from the anti-notch and this is the depinning field that will be described later on.

It is interesting to note that for nanowire having a sloped (model 2) edge profiles, the energy value at ground state (point ‘f’ in energy diagram) is much smaller than that of nonowire having rectangular edge profile (point ‘a’ in energy diagram). In this case, the DW wall was trapped inside the anti-notch for an applied magnetic field of 40 Oe (simulated image ‘g’) and for a further increment of 110 Oe field the DW structure was remained pinned inside the anti-notch and energy values were almost unchanged. Notably, in the case of model 2, upon the application of 130 Oe field the wall structure remained pinned inside the anti-notch, simulated image (i). whereas in the case of
(A) Total energy as a function of normalized magnetization for 160nm width nanowire with transverse up domain wall configuration and symmetric anti-notch for rectangular edge profile (model 1), sloped edge profile (model 2) and tapered edge profile (model 3). The points (a)-(j) represent the significant energy values that changes throughout the energy landscape. For nanowires considering in this investigation, the total energy is always higher for nanowires based on model 1 than that of models 2 and 3.

(B) Micromagnetic simulations illustrating the pinning behavior of a TUP DW (a-j) for nanowires with rectangular (model 1) and sloped (model 2) edge profiles. The magnetic configurations upon the application of magnetic fields for the nanowires with rectangular edge profile (Model 1) were represented by simulated images (a-e) and with sloped edge profile (Model 2) by simulated images (f-j), respectively. These images are corresponding to the marked points in graph (A). In the case of model 1, the DW prior to depin was extended from the anti-notch much more, image (d) than that of wires considering model 2, image (i).

Figure 4.2: Total energy as a function of Normalized Magnetization for TUP domain wall
model 1, upon the application of same amount of field, simulated image (d), the wall structure was extended significantly prior to depin from the anti-notch. Therefore, we may conclude here that if the wire edge of the nanowire is sloped rather than ideal rectangular then prior to depin from the anti-notch the wall structure doesn’t extend rather pinned inside the anti-notch and the magnetostatic energy is also remain almost unchanged. The extension of wall structure prior to depin is an obvious obstacle for energy minimization as well as miniaturization and will be further discussed in detail at the end of this chapter.

Furthermore, for nanowires having sloped edge profile (model 2), the wall structure remained pinned up to an applied magnetic field of 170 Oe and it is depin at 180 field (simulated image ‘j’). The depinning field for nanowire having a rectangular edge profile (model 1) was only 140 Oe, simulated image (e). Therefore, compare to model 1, the depinning field for model 2 is much higher. This ultimately indicates a favorable control of TUP domain wall inside the anti-notch of a nanowire with experimentally observed sloped edge profile.

4.1.2 Energy profiles of vortex domain wall

For a comparatively larger width, 150nm to 300nm, of nanowires the preferred domain wall structure is vortex domain wall (VDW) [102] according to the phase diagram calculated by Nakatani et. al. [6]. It was mentioned earlier that a vortex wall is also identified by the vortex chirality, which can be clockwise or counter clockwise depending on the sense of magnetization rotation about the vortex core.

Figure 4.3 (a) shows schematically a clockwise vortex domain wall (CW VDW) of a planar nanowire along with an a symmetric anti-notch at the middle of the wire. The corresponding magnetization distribution of the CW VDW is shown in the simulated image, figure 4.3 (b). Similarly, counter clockwise vortex domain wall (CCW VDW) and it’s magnetization distribution are shown in figures Figure 4.4 (a) and (b), respectively. In order to obtain a controlled behavior of CW and CCW VDW, we have simulated nanowires of 10 nm Permalloy thickness by varying wire width from 150 nm to 300 nm. The total energy as a function of normalized magnetization for a CW and
Chapter 4

Figure 4.3: (a) Illustration of a nanowire with clockwise vortex domain wall configuration and symmetric diode shaped anti-notch. (b) shows the magnetization directions the relaxed state.

Figure 4.4: (a) Illustration of a nanowire with counter clockwise vortex domain wall configuration and symmetric diode shaped anti-notch. (b) shows the magnetization directions the relaxed state.

CCW vortex domain wall configurations for a representative wire width of $240\,\text{nm}$ with symmetric anti-notch for rectangular (model 1), sloped (model 2) and tapered (model 3) edge profiles are shown in figures 4.5 and 4.6, respectively. The significant energy points inside these curves, figure 4.5A and figure 4.6A, were marked by points (a) to (e) for model 1 and (f) to (j) for model 2. The corresponding simulated images shown in figure 4.5B and figure 4.6B illustrating the pinning behavior of CW VDW and CCW VDW domain wall, respectively, images (a) to (e) for nanowires with rectangular edge profile (model 1) and images (f) to (j) for sloped edge profile (model 2). Notably, these images are corresponding to the marked points in graphs (A) of figures 4.5 and 4.6.

Like TUP domain wall, the total energy as a function of normalized magnetization is again much higher for both CW and CCW VDW in nanowires with a rectangular wire edge (model 1) than that of sloped (model 2) and tapered (model 3) wire edges. Other notable behavior is the extension of domain wall prior to depin from the anti-
(A) The total energy as a function of normalized magnetization for 240 nm wide nanowire with symmetric anti-notch for models 1, 2 and 3. The wall structure is CW VDW. For CW, the total energy is always higher for nanowires having rectangular edge profile (model 1) than that of sloped (model 2) and tapered (model 3) edge profiles.

(B) Micromagnetic simulations illustrating the pinning behavior of a CW VDW (a-j) for nanowires with rectangular (model 1) and sloped (model 2) edge profiles. The magnetic configurations upon the application of magnetic fields for the nanowires with rectangular edge profile (Model 1) were represented by simulated images (a-e) and with sloped edge profile (Model 2) by simulated images (f-j), respectively. These images are corresponding to the marked points in graph (A). In the case of model 1, the DW prior to depin was extended from the anti-notch much more, image (d) than that of wires considering model 2, image (i).

Figure 4.5: Total energy as a function of Normalized Magnetization for CW vortex domain wall
(A) The total energy as a function of normalized magnetization for 240 nm wide nanowire with symmetric anti-notch for models 1, 2 and 3. The wall structure is CCW VDW. For CCW VDW, the total energy is always higher for nanowires having rectangular edge profile (model 1) than that of sloped (model 2) and tapered (model 3) edge profiles.

(B) Micromagnetic simulations illustrating the pinning behavior of a CCW VDW (a-j) for nanowires with rectangular (model 1) and sloped (model 2) edge profiles. The magnetic configurations upon the application of magnetic fields for the nanowires with rectangular edge profile (Model 1) were represented by simulated images (a-e) and with sloped edge profile (Model 2) by simulated images (f-j), respectively. These images are corresponding to the marked points in graph 4.6A. In the case of model 1, the DW prior to depin was extended from the anti-notch much more, image (d) than that of wires considering to model 2, image (i).

Figure 4.6: Total energy as a function of Normalized Magnetization for CCW vortex domain wall
notch of nanowire with a rectangular wire edge as was illustrated in the simulated images (d), figures 4.5B and 4.6B. In the case of nanowires with a sloped edge profile, like TUP wall, the CW and CCW VDW structures did not extend prior to depin from the anti-notch as shown in the simulated images (i), figures 4.5B and 4.6B. The CW and CCW vortex domain wall was found also to pin strongly inside the anti-notch of nanowires with a sloped edge profile. Therefore, obviously the domain wall depinning field was higher for nanowires with sloped edge profile.

It is also to be noticed that the significant energy change point shows exactly same behavior for clockwise and counter clockwise VDW in figures 4.5A and 4.6A. The corresponding behavior of CW and CCW VDW in figures 4.5B and 4.6B is also exactly similar. This clearly indicates that the chirality effect [9, 63, 64, 102] is completely insensitive for symmetric anti-notch. In order to investigate the chirality effect, we have modeled the asymmetric anti-notch as a pinning site for VDW which will be discussed in detail in section 4.5 further in this chapter.

4.2 Total energy at ground state as a function of nanowire width

The behavior of magnetic domain wall in a planar nanowire structure are getting more and more attention with potential applications including both spintronic logic and magnetic memory devices [2, 35, 36, 107]. The stable state of a domain wall is corresponding to a minimum energy point. The total energy at ground state, i.e. just at the relaxed state without applying any magnetic field to move the domain wall, always provides an overview of the minimum energy profile of the system. At ground state the magnetic domains of nanowire rearranges themselves from randomness into a defined DW structure by minimizing the total energy i.e. mainly magnetostatic and exchange energy. So far, the total energy was described as a function of normalized magnetization for some representative wire widths for TUP and CW/CCW VDW. Now we have plotted the total energy at ground state as a function of wire widths for both TUP and vortex domain wall. The variation of ground state energy as a function of wire
widths is shown in figure 4.7. In the graph the solid symbols are representing TUP domain wall in nanowire with rectangular (model 1), sloped (model 2) and tapered edges (model 3), respectively. Similarly the open symbols are representing the same for VDW. The variation of ground energy is obviously higher for wider nanowires but the notable point is that for any wire width the energy at ground state is much smaller for nanowires having sloped and tapered edges compared to that of rectangular edge profile. For a reliable operation of DW based devices, a stable state of DW with minimum energy at ground state is desired and this can be achieved if the wire edge is like experimentally observed sloped or tapered edges.

![Figure 4.7: The energy values at ground state as a function of wire width for nanowires of different edge profiles. In figure, solid symbols correspond to TUP DW while open symbols correspond to CCW VDW. Notably, the energy values for CW and CCW VDW are same as the anti-notch is symmetric. The total energy values at ground state as for different wire widths are higher for nanowires with rectangular edge (model 1) than that of sloped and tapered edge (models 2 and 3, respectively).](image)

Section 4.3
4.3 Total energy prior to depin as a function of wire width for symmetric anti-notch

Total energy prior to depin is the maximum energy up to which the domain wall remain trapped inside the pinning site, i.e. inside the anti-notch in this investigation. We have calculated the total energy prior to depin for different nanowire widths by placing a symmetric anti-notch as pinning site at the middle of the wire. The total energy prior to depin the TUP and VDW from the anti-notch was plotted as a function of wire width, figure 4.8. For symmetric anti-notch the energy values are same for clockwise and counter clockwise VDW as was also mentioned earlier. Figure 4.8 shows that the total energy prior to depin from the anti-notch increases more or less linearly with the increase of nanowires width. The energy prior to depin the DW from the anti-notch of nanowire with rectangular edge profile (model 1) than that of sloped and tapered edge profiles (models 2 and 3, respectively).

![Figure 4.8: The energy values prior to depin the TUP and CCW VDW from symmetric anti-notch as a function of wire width for nanowires of different edge profiles. In figures, solid symbols correspond to TUP DW while open symbols correspond to ccw VDW. The energy values prior to depin the DW are much higher for nanowires with rectangular edge profile (model 1) than that of sloped and tapered edge profiles (models 2 and 3, respectively).](image)

Section 4.3
extension or distortion of the wall structure. We have observed such an extension of the DW structure from our simulated images (d) of figures 4.2A and 4.5B. This is quite unexpected for a controlled pinning and depinning of a domain wall. From the plot, figure 4.8, it is also noticeable that for model 1 i.e. for nanowires with rectangular edge profile; the energy landscape shows some random behavior for vortex domain wall configuration. This randomness was found to eliminate if the wire edge is sloped or tapered. In the proposed spintronic devices, the movement of the domain wall will be controlled by geometrical pinning site upon the applied magnetic field [35, 36]. The field required to depin a DW from the anti-notch actually indicates the pinning strength of that anti-notch and this is referred as domain wall depinning fields. In the next stage of this investigation we will discuss depinning field as a function of wire width in nanowires having standard rectangular as well as experimental sloped and tapered edge profiles.

4.4 Depinning field as a function of wire width for symmetric anti-notch

The ability to control precisely the motion of magnetic domain walls in ferromagnetic nanowires is crucial for future realization of proposed magneto-electric (or spintronic) devices [37, 107] as well as for greater understanding of fundamental nanomagnetic behavior [20]. Relationship between the depinning field and pinning site geometry is highly relevant to field driven domain wall behavior and crucial to optimize the efficiency of the domain wall based devices. The DW depinning field i.e. the field required to move the DW from the pinning site ultimately indicates the strength of this pinning potential as was mentioned earlier. The domain wall depinning field as a function of nanowire width for all three models were calculated from micromagnetic simulations and are presented in figure 4.9. From the plot it is shown that the depinning field decreases with increase of nanowire width. This is in a good agreement with findings by L. K. Bogart et. al. [64] for planer Permalloy nanowires. It is noteworthy that the domain wall depinning field, that is the strength of the pinning potential of a particular
nanowire with a particular anti-notch is again higher if the wire edge is either sloped or tapered rather than rectangular which is considered ideally in all micromagnetic simulations performed so far. This phase diagram of domain wall depinning field versus wire width, figure 4.9, also demonstrates that for nanowires with sloped or tapered edge profiles, the domain wall depinning field is much higher for wire widths 120 nm to 240 nm. Notably, even by using the most advanced fabrication techniques [9] it is difficult to fabricate well defined nanowire with wire width around 100 nm. However, fabrication of wider nanowire comparatively easy but not preferable from the storage density point of view. Our results indicates, figure 4.9, nanowire of width ranging from 120 nm to 240 nm shows higher pinning strength for both TUP and VDW configuration for nanowires with experimentally observed sloped and tapered edges. This actually indicates a preferred range of nanowire width for device applications. In the next stage of this investigation, we will describe the chirality effects of domain walls.
4.5 Chirality effect of domain walls

The interaction of DW with geometric features doesn’t depend only on the feature geometry but also on the chirality of the incoming DW’s [9, 63, 64, 102]. As was mentioned earlier for symmetric anti-notch the chirality dependence is insensitive. It was reported that different domain wall structures will experience different pinning interactions with a single notch structure [10, 64, 108, 109], since the spin configuration through a structurally asymmetric feature presents different energetic barriers to a domain wall traveling through the anti-notch. This energetic difference manifests itself as a difference in the magnetic field required to push the wall through a structural pinning feature, in our case diode shaped anti-notch. Therefore, to explore how DW of different chiralities (clockwise and counter clockwise VDW) interact with an asymmetric anti-notch, we have modeled here asymmetric anti-notch along the nanowires with different edge profiles. Figures 4.10 and 4.12 illustrate the energy landscape of

![Graph](image-url)

Figure 4.10: The total energy as a function of normalized magnetization for 240 nm wide nanowire with rectangular (model 1), sloped (model 2) and tapered (model 3) edges. The wall structure is clockwise and the anti-notch is asymmetric. The points (a)-(j) represent the significant energy values that changes throughout the energy landscape. The total energy is always higher for nanowires with rectangular edges (model 1) than that of wires with sloped and tapered edges (models 2 and 3, respectively).
Figure 4.11: Micromagnetic simulations illustrating the pinning behavior of a CW VDW (a-j) for nanowires with rectangular (model 1) and sloped (model 2) edge profiles. The magnetic configurations upon the application of magnetic fields for the nanowires with rectangular edge profile (Model 1) were represented by simulated images (a-e) and with sloped edge profile (Model 2) by simulated images (f-j), respectively. These images are corresponding to the marked points in graph, figure 4.10. In the case of model 1 and model 2, the CW DW prior to depin from the anti-notch was pinned inside the anti-notches, images (d) and (i), however the pinning strength was higher for model 2 compared to model 1.

clockwise and counter clockwise vortex domain wall configurations for a representative wire width of 240 nm with asymmetric anti-notch for rectangular (model 1), sloped (model 2) and tapered (model 3) edges. The significant energy points inside these curves, figure 4.10 and figure 4.12, were denoted by points (a) to (e) for model 1 and (f) to (j) for model 2. The corresponding simulated images shown in figure 4.11 and figure 4.13 illustrating the pinning behavior of CW VDW and CCW VDW domain wall, respectively, images (a) to (e) for nanowires with rectangular edge profile (model 1) and images (f) to (j) for sloped edge profile (model 2). Notably, these images are corresponding to the marked points in the graphs of figures 4.10 and 4.12. As was observed for TUP, CW/CCW VDWs in nanowires with symmetric anti-notches, the total energy values are again higher for nanowires having a rectangular edges. This is demonstrated in figures 4.10 and 4.12. Again from energy minimization point of view, the favorable behavior is observed for nanowires with sloped and tapered edge profiles even the anti-notch structure is asymmetric. But here the notable point is that for CW VDW, the domain wall inside the anti-notch is pinned strongly without extending the structure from the anti-notch, images (d) and (i) of figure 4.11. The leading part
Figure 4.12: The total energy as a function of normalized magnetization for 240 nm wide nanowire with rectangular (model 1), sloped (model 2) and tapered (model 3) edges. The wall structure is counter clockwise and the anti-notch is asymmetric. The points (a)-(j) represent the significant energy values that changes throughout the energy landscape. The total energy is always higher for nanowires based on model 1 than that of models 2 and 3.

Figure 4.13: Micromagnetic simulations illustrating the pinning behavior of a CW VDW (a-j) for nanowires with rectangular (model 1) and sloped (model 2) edge profiles. The magnetic configurations upon the application of magnetic fields for the nanowires with rectangular edge profile (Model 1) were represented by simulated images (a-e) and with sloped edge profile (Model 2) by simulated images (f-j), respectively. These images are corresponding to the marked points in graph, 4.12. In the case of model 1, the DW prior to depin was extended from the anti-notch much more, image (d) than that of wires with sloped edge (model 2), image (i).
of the VDW has a component parallel to the magnetization of the anti-notch directed from right to left; therefore, the VDW is strongly pinned inside the anti-notch.

On the contrary, for CCW VDW, the domain wall inside the anti-notch does not pin upon the application of a magnetic field of 30 Oe, rather the wall structure starts to extend further from the anti-notch, images (b) and (g) of figure 4.13. For a further increment of the field, the wall structure from the anti-notch extended significantly, images (d) and (i) of figure 4.13. The corresponding energy values in each point was much higher for CCW VDW (figure 4.12) than that of CW VDW (figure 4.10). Therefore, the simulated images, figure 4.11 and figure 4.13 clearly demonstrate that for asymmetric anti-notch the CW VDW pinned inside the anti-notch, whereas the CCW VDW extend further from the anti-notch prior to depin. We can conclude definitely that for an asymmetric anti-notch fabricated along the upper side of a nanowire the favored wall chirality is clockwise. This actually indicates the chirality sensitivity of the anti-notch. If we compare this behavior for nanowires with rectangular, sloped and tapered edge profiles then considering energy values and pinning strength we can obviously say that the favorable behavior of domain wall is again observed if the wire edge is modeled according to experimentally observed edge profiles of the nanowires.

Prior to summarize our results in Chapter 5, the complete data for domain wall extension observed in this investigation are presented in the tables 4.1 and 4.2 for transverse up and vortex domain wall, respectively. From table 4.1 it is evident that

<table>
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<th>Wall Width</th>
<th>Wall Type</th>
<th>Wall Extension in nm</th>
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</thead>
<tbody>
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<td></td>
<td>Model 1</td>
</tr>
<tr>
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<td>15</td>
</tr>
<tr>
<td>110</td>
<td></td>
<td>110</td>
</tr>
<tr>
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Table 4.1: The table shows the extension of the TUP from symmetric anti-notch of nanowires with varying width and edge profiles. The wall extension is much higher for nanowires with rectangular edge (model 1) profiles that that of sloped (model 2) and tapered (model 3) edge profile.

the domain wall extension is a dominant feature for nanowires with rectangular edge
profile (model 1). For narrower wire widths (less than 120 nm) which are very difficult
to fabricate in real practice, the wall extension between different models does not differ
significantly. However, from wire width 120 nm the wall structure prior to depin extend
significantly if the wire edge is model according to ideal consideration which is like a
rectangular cross-section of a nanowire. Notably, for 180 nm wide nanowire, we did
not observe any extension of the domain wall. Actually, from domain wall structure
phase diagram [6] it is very unlikely to form a TUP domain wall if the wire width is 180
nm and film thickness is 10 nm. Therefore, for this wire width and thickness a stable
wall structure do not form and they do not extend. The extension of domain wall of

Table 4.2: The table shows the extension of the CW and CCW VDW from symmetric as well as
asymmetric anti-notches of nanowires with varying width and edge profiles. The wall extension is
much higher for nanowires with rectangular edge (model 1) profile that of sloped (model 2) and
tapered (model 3) edge profiles.

<table>
<thead>
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<th>Cholarity</th>
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<td>CW</td>
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both CW and CCW chiralities prior to depin from the symmetric and asymmetric anti-
notches are shown in Table 4.2. The wall structure does not extend if the anti-notch

Section 4.5
is asymmetric and the chirality of the incoming domain wall is CW VDW. On the contrary, the CCW VDW extends significantly from the asymmetric anti-notch. For symmetric anti-notch, the wall extension of CW and CCW VDW is same and much higher if the wire edge is rectangular. For sloped and tapered edge, the wall extension for different wire widths is either absent or insignificant as shown in table 4.2. In the next chapter we will summarize the results of this investigation and will present the concluding remark along with the motivations for future work.
Chapter 5

Conclusion & Future Work

5.1 Summary of this investigation

We can summarize the results of this investigation as follows:

(1) Total energy of the nanowire as a function of normalized magnetization shows that for nanowires with rectangular edge profile, the total energy is significantly higher than that of nanowires with sloped and tapered edge profiles, for all type of domain wall configurations, i.e. TUP, clockwise VDW, counter clockwise VDW. At ground state as well as prior to depin the DW from the anti-notch the energy is higher for nanowires with rectangular edge compared to that of nanowire with experimentally observed edges. Notably, depinning energy is a vital point for controlling domain wall motion through pinning sites in the nanowire. In spintronic devices, the digital data bit is recorded by trapping of a domain wall at geometrical pinning sites in nanowire. The data read write operation depends on domain wall movements through the nanowire which is done by pushing the domain walls inside the nanowire by applying magnetic field. Therefore, for a reliable operation of domain wall based devices, energy minimization is expected and this is achievable in nanowires having sloped and tapered edge profiles rather than in ideal nanowires having a rectangular cross-section of the wire edge.

(2) The domain wall depinning fields were calculated for different wire widths by varying the edge profiles of TUP and VDWs. The domain depinning fields were
decreased for higher wire widths and is in good agreement with previous investigation [64]. The outcome of our micromagnetic simulations revealed clearly that the depinning fields are significantly higher over a wide range of wire width (120nm - 240nm) along the nanowires of sloped and tapered edge profiles. In this region, the depinning field i.e. pinning strength is much higher if the wire edge is sloped or tapered. It is well known that fabrication of narrower nanowire compared to the width of domain wall (100nm) is very difficult even using most advanced nanofabrication techniques. For higher density data storage point of view, the wire width above 250nm is not preferred. Within this preferred dimension (120nm - 240nm and a Py thickness of 10nm) of the nanowire, the domain wall behavior considering energy values and pinning strength is favorable if the wire edge is according to experimentally observed edge profiles.

(3) For asymmetric anti-notch the influence of edge profile on the chilarity effect of VDW was clearly identified. It is found that for asymmetric anti-notch the favorable chirality is clockwise VDW. In clockwise vortex domain wall configuration the pinning behavior is much more precise and the domain wall confinement inside the pinning site is much more stable. The leading part of the VDW has a component parallel to the magnetization of the anti-notch directed from right to left; therefore, the VDW is strongly pinned inside the anti-notch. On the other hand, counter clockwise VDW domain wall shows large extension prior to depin completely from the pinning site. Notably, for both chiralities (CW/CCW VDW), the energy value is minimized if the wire edge is sloped or tapered. The chilarity effect also demonstrates that the favorable chirality for asymmetric anti-notch is clockwise VDW if the anti-notch is fabricated in the upper side of the nanowire. Furthermore, the counter clockwise VDW will be a favorable chilarity for asymmetric anti-notch considering mirror symmetry of the nanowire geometry if the anti-notch is fabricated in the lower side of the nanowire as shown in figure 5.1(b) (iii). The desired chirality of the DW is possible to form in real practice [9]. Therefore, by fabricating asymmetric anti-notch alternatively along the favorable orientation of the nanowire i.e. alternatively in the upper side and
lower side of the nanowires we can design the orientation of the anti-notch and arrangement of the nanowires in a DW based device that will perform higher storage density. This is shown schematically in Figure 5.1.

![Figure 5.1](image_url)

Figure 5.1: (a) Schematic illustration of a conventional design of the orientation of the anti-notch and arrangement of nanowires to utilize the favorable chirality effect. In Figure 5.1 (a), the anti-notch will be fabricated along the upper side of the nanowire and the nanowire will be arranged in parallel and the chirality of the incoming DW will be clockwise. On the contrary, in Figure 5.1 (b), the anti-notch will be fabricated in the opposite sides of two nanowires and the nanowires will be arranged alternatively. For Figure 5.1 (b) (iii), the favorable chirality will be CCW VDW where for Figure 5.1 (b) (iv), the favorable chirality will be CW VDW. The width i.e the area required for arrangement (b) is lower than that of (a) designated by h and H, respectively. This will enhance the storage capacity.

(4) Domain wall extension was found for nanowires with rectangular edge profile whereas with sloped and tapered edge profile the wall extension is either absent or insignificant. This wall extension in nanowire with rectangular edge corresponds to a higher energy state mainly of magnetostatic energy. The confined pinning of domain wall inside pinning site and depinning without extension refers to the efficient read write operation in spintronic memory or logic devices. The domain wall extension prior to depin introduce a spatial uncertainty in domain wall motion which reflects poor read write performances. Domain wall extension also causes low density of usable pinning sites which might effect directly the data density in spintronic memory devices.

5.2 Conclusion

The TEM cross-sectional images demonstrated clearly that using both EBL and FIB techniques well defined edge profiles are possible to produce in nanowires. The results
of our micromagnetic simulations reveal the favorable behavior of the domain walls in nanowires with tapered and sloped edge profiles. The tapered or sloped edges certainly have an effect due to the effective variation of nanowires width. In the case of vortex domain wall, we also believe that nucleation of wall also effects for example the vertices also changes significantly with the sloped or tapered edge compared to the flat rectangular (vertical) edge. The question which might arise now is that can we deliberately produce nanowires with tapered or sloped edge profiles? It is certainly possible to pattern nanowires of tapered edge profiles using EBL technique if bi-layer PMMA resist is used during pattern generation. More than twenty cross-sectional TEM images were captured from a number of EBL patterned nanowires and each time a tapered edge profile of those nanowires were observed [9]. In the case of FIB patterned nanowires the edge profiles of the nanowires were also mostly tapered, however, a small percentage (less than 20 %) of them are sloped. Interestingly a recent investigation of another research group also demonstrates clearly that the edge profiles of the FIB patterned cobalt nanowires are tapered [14]. The rich diversity of their behavior reported here using micromagnetic simulations highlight the new definition of the edge profiles which are either tapered or sloped. This is evidently in accordance with experimental observations, however, notably distinct from ideal and mostly used considerations particularly in micromagnetics simulation.

5.3 Future Work

Object Oriented Micro Magnetic Framework (OOMMF) is widely used in micromagnetics simulation to study magnetic behavior. It is highly accurate and can represent visually the magnetic states in designated steps. However the main cons of this program that it takes significant amount of time calculating a single step. Though not all the steps takes equal time but those involves multiple magnetic interaction took large amount of time. To speed up we have to use multicore or multiprocessor environment. Although OOMMF can be used in multicore or multiprocessor system by using threaded TCL software and defining OOMMF_THREADS environment variable while using ”oxsii or boxsi” solver. But the implementation of multithreading in
OOMMF seems like using OpenMP directives implementation. OOMMF code is aware of OpenMP directive which can only be activate by compiling the OOMMF package with a threaded version of $TclTk$ implementation. OpenMP provides some code optimization like loop unrolling, lock synchronization, no loop code, parallel looping etc. OpenMP generally implement multithreaded task distribution between all available code in a very general fashion. By manually optimizing code can always gives us outstanding performance increase. Combining manual optimization with OpenMP sometime gives even better result. For a very large problem where the number of cell is the sample is substantially large even a multicore system can be a bottleneck. In such scenario a multinode cluster environment is perfect candidate for parallel processing.

Another new emerging parallel processing technology is GPU computation or widely known as General Purpose Graphics Processing Unit (GPGPU). Modern graphics card is massively parallel processing system that follows embarrassingly parallel architecture for boosting parallel processing in a superscaler fashion. Generally a conventional CPU (Central Processing Unit) in our workstation/server has 4 to 12 processing core which can be used in parallel for multithreading. But a standard GPU can have thousands of processing cores. Although each core in a GPU is much slower than the conventional CPU but containing thousands of core working in parallel sometime outnumber the computational performance of conventional CPU in an exponential scale. The only problem with GPGPU is that it is not suitable for all type of computation problem. GPGPU particularly suitable for embarrassingly parallel computation where no data sharing is required among different processing unit after data domain distribution. Cutting edge GPU technology allows more efficient data communication between processors than their predecessors but still they are very much outperform by conventional CPU in this regard.

So, I would like to work further with OOMMF to increase the computation performance of the code. My idea is to optimize manually the OOMMF kernel code to boost up the calculation performance. Next step of optimizing can be done by implementing OpenMPI, a open source implementation of Massage Passing Interface, programming architecture to use multi-node cluster to scale up the calculation performance of
OOMMF. OpenMPI can also be used carefully with OpenMP, if applicable, to speed up even more. Finally, the final step of speed up can be done using GPU for computation. Implementing GPGPU processing with CUDA or OpenCL, two competing technology to use GPU for general purpose processing might allow us achieve tremendous performance increase. Using python, a platform independent modern scripting language, the domain data can be distributed among multiple nodes so that they can be processed in parallel completely independent of each other or with as minimum data sharing as possible.

Optimizing code may seems like the domain of computer sciences but in a physics simulation software like OOMMF the code performance is not as much priority as the accuracy of the code. Optimizing code can dramatically increase code performances with the cost of accuracy of the calculation. This is embedded in the fundamental limitations of computers, the approximate representation of floating point number in computer memory and floating point asthmatics. So, optimizing a scientific code like OOMMF must maintain high computation performance within the tolerant limit of computational accuracy for which understanding the physics is as much important as understanding the software code for implementation of numerical solutions for the given problem. On the other hand optimization also results in faster calculation which gives us a opportunity to go further to the high granular level while designing micromagnetic simulations with OOMMF. As the computation time is reduced a smaller cell size, viz. 1 nm cell size, can be used to achieve more precise edge profiles of the nanowires.
Appendix A

Complete simulation process

This section discusses the complete simulation process, centered around the diagram in figure E.1. This diagram shows the major supporting libraries, compilers, interpreters, scripts, data stores and outputs of the method.

A.1 Notation

- Ellipses with purple text show an intermediate data set necessary for combining components together.

- Boxes with blue text indicate a complex custom application designed to convert or otherwise handle the input and output of one application or library.

- Ellipsoids with red text show a supporting external application necessary for visualization, pre or post-processing or run-time.

OOMMF is available from the NIST website as either a source code package with a straightforward build process or as a pre-compiled binary application for many architectures and operating systems, such as GNU/Linux or Microsoft Windows. The framework of the three-dimensional micromagnetic problem solver, Oxs (the OOMMF Extensible Solver), is shown in figure E.2. The blue items in boxes here show areas which can be straightforwardly extended to include, for example, a twenty-six neighbor exchange energy contribution rather than the standard six neighbor ex-change provided
Figure A.1: The OOMMF extensible solver framework. Blue items in boxes indicate extensible areas as standard with OOMMF. Oxs provides a powerful mechanism for extending this micromagnetics package.
Bibliography


