Computational and Experimental Research
in Materials and Renewable Energy (CERiMRE)
Volume 8, Issue 1, page 89-97
eISSN : 2747-173X

Submitted : May 10, 2025
Accepted : May 30, 2025
Online : May 31, 2025
DOI :10.19184/cerimre.v8i1.53697

Study of Magnetic Features of NiFe Feromagnetic Materials at Various Composition Variations by Simulation Methods

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Abstract. *This study aims to evaluate the effect of composition on the Curie temperature (Tc) value and examine the impact of temperature on the hysteresis curve and magnetic properties of NiFe ferromagnetic materials. The methods used include molecular dynamics to calculate the exchange interaction value (Jij) and the Monte Carlo method to determine the Tc value. Simulations were carried out on various compositions of NiFe material to obtain a complete picture of its magnetic properties. The simulation results show that the $Ni_{10}Fe_{90}$ composition with a cube structure has the highest Tc value, 660 K, while in the sphere structure, Tc reaches 620 K. The magnetization value of the material decreases with increasing temperature and approaches zero when approaching the Curie temperature. Meanwhile, the susceptibility value has a low value at low temperatures, increases to reach the maximum value at Curie temperature, and decreases thereafter. The decrease in susceptibility value after reaching Curie temperature indicates a change in the phase of the material from ferromagnetic to paramagnetic. These findings are significant as they provide a deeper understanding of the behavior of NiFe ferromagnetic materials at different temperatures. Other observations were made to analyze the hysteresis curve. The results obtained from the hysteresis curve show a magnetic saturation value of 1 and an easy axis located on the z-axis, with a coercivity field of 0.05 Oe. In conclusion, NiFe material with $Ni_{10}Fe_{90}$ composition shows optimal magnetic performance at high temperatures, making it a promising candidate for applications in certain thermal environments. This study provides important insights into the relationship between the composition, structure, and magnetic properties of NiFe materials, as well as the implications for the development of more efficient ferromagnetic materials.*

Keywords: NiFe, Curie Temperature, VAMPIRE, Exchange Interaction, Ferromagnetic

Introduction

The development of technology today requires humans to quickly adapt, one of which is a computer. Currently, computers require large storage media but with a small size or commonly known as a hard disc drive (HDD). The hard disk drive (HDD) will reach a temperature of 30°C to 50°C when the computer is turned on and the temperature will increase to 58°C when the computer is used. The hard disk drive will be permanently and irreversibly damaged when the temperature reaches 66°C [1]. According to [2], a hard disk drive has main components including a disc that functions to store data magnetically, a read/writehead that functions to read and write data on the disc, a slider that functions where the head is mounted and a shield that functions to control the magnetic field and protect sensitive elements. According to [1], HDD will suffer permanent and irreversible damage when the temperature has reached 66°C and according to damage to HDD is generally caused by high asperity, corrosion, scratches, and contamination which are all affected by the quality of the protective surface. Materials that can be used to make

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HDD and minimise damage are materials that have unidirectional magnetic properties and have high heat resistance. The materials that have these properties are ferromagnetic materials and some examples of materials include iron (Fe), nickel (Ni), cobalt (Co), and their alloys [3].

Ferromagnetic material is a type of material that has strong magnetic properties due to exchange interactions between atomic magnetic moments. These properties cause the magnetic moments to align and produce spontaneous magnetisation even though the external magnetic field is removed [4]. The basic properties of ferromagnetic materials include spontaneous magnetisation, magnetic domain, hysteresis curve, coercivity, and high magnetic permeability [5]. One of the important characteristics of ferromagnetic materials is the hysteresis curve or the relationship between magnetisation and the external magnetic field, including the coercivity and remanence values which are indicators of the strength and stability of the magnetisation of the material [6]. The hysteresis curve of a ferromagnetic material can be obtained by graphing the magnetisation of the material (M) against the applied magnetic field strength (H) or the magnetic field induction (B) against the magnetic field strength (H) [7]. Spontaneous magnetisation possessed by ferromagnetic materials can be characterised by the presence of electron spin and magnetic moment.

NiFe material is currently being developed for technology because this material is suitable for application to objects that require sensitive and efficient magnetic response because it has high permeability and low coercivity field [8]. The characteristics of this NiFe material include saturation magnetisation (Ms) of $8x10^5$ A/m, exchange constant (A) of $12x10^{-12}$ [9] and anistropy constant (K) of $0.5x10^3$ [10]. This material is often used because it has unique properties including the FCC crystal structure at temperatures above 910°C [11] then around 1390°C the structure will return to BCC and melt at a temperature of 1535°C [12], but on the other hand the crystal structure of nickel is FCC with a melting point of 1445°C. Other properties include not reacting with air, resistance to oxidation, and can maintain properties at high temperatures [13].

Micromagnetic simulation has become one of the important methods to understand the characteristics of magnetic properties of NiFe ferromagnetic materials. The principle of this simulation is to involve a model of magnetisation dynamics at a microscopic scale to understand the behaviour of the magnetic domain and the response of the material to an external magnetic field. Computational methods have emerged as an important method in researching ferromagnetic materials, as they can effectively capture the microscopic characteristics of materials without relying significantly on complicated and expensive experiments. In the NiFe material domain, simulation serves to examine the magnetisation values, spin interactions, and magnetic domain behaviour regarding changes in external magnetic field and temperature. One software with an atomistic spin model and allowing visualisation of magnetisation dynamics at the atomic level is VAMPIRE [14]. In addition, this simulation can also be used to see the magnetic performance affected by variations in composition and crystal structure [15]. Furthermore, further research has examined alloy materials and offered insights into magnetic properties including magnetic anistropy and hysteresis curves using atomistic micromagnetic simulations [9].

Theoretical Background

The simulation requires consideration of key parameters to ensure accurate modeling of magnetic behavior. The magnetic properties of ferromagnetic materials are influenced by several factors including the magnetic spins between atoms which are intrinsic properties of particles that function

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to create magnetic moments [16]. The magnetic moments of neighbouring spins tend to align and are driven by a quantum effect commonly known as the exchange interaction. These interactions are used to arrange the spins into magnetic domains that will produce magnetisation. However, these spins will move freely when the material has reached the curie point (Tc) or critical temperature of the material which causes the loss of spin alignment and the material will switch phase to paramagnetic. However, when the magnetic field is removed, the material will retain residual magnetisation which causes a delay in the material's response to not being magnetised. This condition is commonly known as a hysteresis curve and can be determined by analysing using a loop-shaped hysteresis curve.

Simulation of Magnetic Properties of NiFe Materials

This simulation is carried out through three main stages, namely the determination of exchange interaction parameters using LAMMPS, simulation of material magnetic properties using LAMMPS, and analysis of simulation results to obtain magnetic properties including curie temperature and hysteresis curve. In the first stage, simulations were carried out using LAMMPS to vary the atomistic structure of NiFe material from $Ni_{10}Fe_{90}$ to $Ni_{90}Fe_{10}$ composition. The output obtained from the LAMMPS simulation is then extracted to obtain the exchange constant value. The second stage is a simulation using VAMPIRE to calculate magnetic properties at the micromagnetic scale. This simulation is carried out by providing an external magnetic field and temperature to obtain magnetisation dynamics which will produce data for hysteresis curves and curie temperatures. The third stage is data analysis of the simulation results to determine the effect of composition variations on changes in temperature, magnetic moment and hysteresis curve. The analysis carried out at this stage is also carried out by visualising using origin and pov ray. This stage is important to understand the relationship between the parameters and the behaviour of the magnetic properties of the material.

Materials and Methods

In this study, simulations were carried out using LAMMPS with the molecular dynamics method and VAMPIRE with the monte carlo method. Both methods are approaches in computing that complement each other in studying magnetic properties. The software used in this simulation includes LAMMPS for atomistic simulation, VAMPIRE for micromagnetic simulation, python for data processing, origin for data analysis, and POV-RAY for visualisation of simulation results. The simulation materials used include LAMMPS input data, EAM potential data, VAMPIRE input files and material files, and UCF files obtained from the extraction of LAMMPS output data.

The technical parameters used in this study are:

- LAMMPS simulation:
    - Face centreed cubic (FCC) crystal structure.
    - Box size: 5x5x5
    - Lattice parameters: 3.54 Å
    - Temperature: 100 °C
- Curie temperature and hysteresis curve with VAMPIRE:
    - Temperature 0K-1600K with 20K interval to find curie temperature and 0K for hysteresis curve.
    - System dimension 5 nm

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- External magnetic field 2T

The exchange interaction value is obtained from extracting total energy data on several atomic configurations and calculating the energy difference obtained when the spin is changed. These values are then converted into Jij parameters by considering the Heisenberg model. The process allows for calibration of the exchange interaction values to suit the structure and simulation conditions. The value obtained is then used for micromagnetic simulation purposes. In addition, the use of 100°C temperature in the LAMMPS simulation aims to explore the upper limit of NiFe material performance under extreme conditions. Although according to [1] HDD will be permanently damaged at 66°C, a temperature of 100°C is used to thoroughly understand the thermal stability of the material.

Results and Discussion

Simulation Setup and Atom Count

This section presents the simulation results of NiFe materials with various compositions and temperatures to analyse their magnetic properties. This simulation is performed using LAMMPS to obtain the exchange interaction value and VAMPIRE magnetic simulation. In the LAMMPS simulation, several parameters have been determined including a lattice parameter of 3.54 Å, a box size of 5x5x5 with an FCC crystal structure which will produce a total of 500 atoms because the FCC crystal structure has 4 atoms in each unit cell. The choice of NiFe material is because the material is widely used for basic materials for making HDDs and has high permeability. In addition, the provision of a temperature of 100°C in the LAMMPS simulation aims to provide more insight into the performance of the NiFe material under high temperature conditions even though the HDD will experience damage at 66°C.

Curie Temperature Analysis

Curie temperature is a critical temperature where ferromagnetic materials can lose their magnetic properties and turn into paramagnetic materials. The curie temperature value in NiFe material is strongly influenced by the composition and spin interaction between atoms. One way to determine the curie temperature value of the material is by relating the susceptibility value to temperature. **Figure 1** shows the relationship between susceptibility and temperature with a cube shape, where there is a decrease in the curie temperature value as the composition of Ni increases. The decrease in curie temperature value is caused by the weakening of the exchange interaction between electron spins, because Fe atoms have a stronger exchange interaction than Ni. In addition, the average magnetic moment of the material also decreases, considering that Fe has a larger magnetic moment than Ni. As a result, the magnetic order is more easily disturbed by thermal energy, so the transition from ferromagnetic to paramagnetic occurs at lower temperatures.

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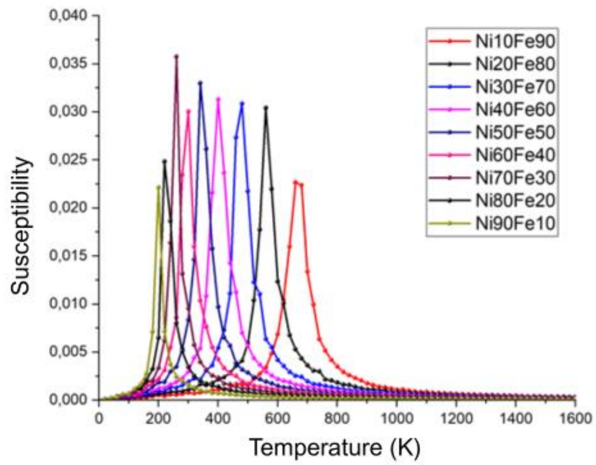

Figure 1. Graph of susceptibility relationship to temperature in each composition variation with cube shape

Susceptibility and magnetisation values play an important role in determining the curie temperature of magnetic materials. Susceptibility is a measure of the degree to which a material responds to a given external magnetic field. The susceptibility value is relatively small when the material is at a low temperature due to the strong interaction and magnetic moment of the material in a regular state. Thermal energy that disturbs as the temperature increases causes a change in the direction of the spin until the susceptibility value increases at the maximum point or curie point. The susceptibility value will decrease after reaching the maximum point due to the weakening of the spin interaction which makes the material undergo a phase change from ferromagnetic to paramagnetic. Conversely, magnetisation will have a maximum value caused by spin alignment when the temperature is low. Thermal energy that continues to increase with increasing temperature results in disturbances in spin orientation and the magnetisation value decreases. When the material reaches the curie temperature, the magnetisation value decreases dramatically to near zero because the thermal energy is greater and causes random magnetic moments.

Hysteresis Curve (Field & Temperature Variation)

Hysteresis curve is one of the characteristics in ferromagnetic materials that shows the change in magnetisation when the magnetic field is increased, decreased, and reversed. Material properties such as magnetic anistropy, exchange interactions, and magnetic domains can affect the shape of the hysteresis curve where magnetic materials that have a wide hysteresis loop indicate a large field to reverse magnetisation and a high coercivity field and conversely a narrow hysteresis loop indicates the material has a low coercivity field and is easy to undergo changes in magnetisation. The hysteresis curve of NiFe material with $Ni_{10}Fe_{90}$ composition shows different characteristics based on the direction of the crystal axis. The results of the hysteresis curve formed when the magnetic field is applied in the direction of the x,y,z axis can be seen in the **Figure 2**.

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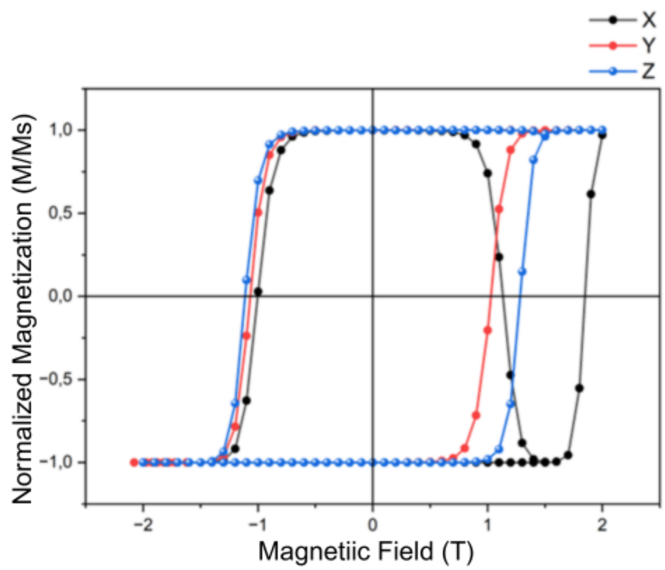

Figure 2. Hysteresis curve of $Ni_{10}Fe_{90}$ material on x,y,z axis

$$H_c eff = \frac{(H_{c+})+(H_{c-})}{2} \quad (1)$$

Using formula (1), the coercivity field values obtained from the simulation on the x,y,z axis are 1.10 Oe, 1.00 Oe, 0.05 Oe respectively and make the z axis as the easy axis of the NiFe material to be easily magnetised. On the contrary, the hard axis is the axis of NiFe material that causes magnetisation to be difficult to align and is located on the x-axis which can be indicated by the non-formation of hysteresis loop. On the y and z axes, there is a similar hysteresis loop shape but different widths with the z axis having a wider shape than the y axis due to the energy required for the magnetisation to reverse direction being quite large. In other compositions, the value of the coercivity field is also analysed and it is found that the compositions that have the lowest coercivity field in the same axis direction besides $Ni_{10}Fe_{90}$ are $Ni_{50}Fe_{50}$ and $Ni_{60}Fe_{40}$, which are 0.5 Oe.

In addition to composition variations, temperature variations are also analysed to obtain changes in coercivity field, remanent magnetisation, and magnetic saturation. The hysteresis curve of $Ni_{10}Fe_{90}$ material on the z-axis with temperature variation can be seen in **Figure 3**. The temperatures used are 0K, 300K, and 600K and produce values of coercivity field and remanent magnetisation that decrease with increasing temperature which indicates that thermal enhancement can disrupt the regularity of magnetic moments. However, the saturation value will be constant at 1 Oe at all temperature variations because saturation magnetisation is not affected by temperature.

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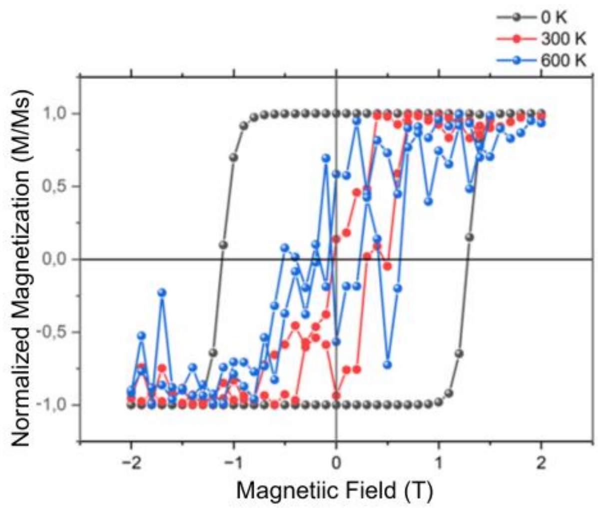

Figure 3. Hysteresis curve of $Ni_{10}Fe_{90}$ material on z axis with temperature variation

Exchange Interaction (Jij)

The exchange interaction value of NiFe material is obtained by performing LAMMPS simulation with composition variation and box size variation. The interaction values obtained are then used as input in the VAMPIRE simulation to further analyse the magnetic properties. The results obtained from the LAMMPS simulation based on composition variations do not follow a regular trend. The irregularity is caused by the influence of the local environment of atoms in the material as well as the effect of magnetic transitions that occur in NiFe materials.

Meanwhile, the variations used to find the exchange interaction value based on the box size are 3.5; 5; 6.5; 8; 8.5 and 11.5. The result obtained from the simulation based on the box size is that the exchange interaction value is getting bigger along with the size of the box used. This indicates that the box size has a significant influence on the resulting exchange interaction value. These results are likely due to the statistical effects of the number of atoms in the system and the length of the spin interaction in the simulation.

Conclusions

LAMMPS-based magnetic simulations and VAMPIRE-based micromagnetics to determine curie temperature values and magnetic properties have been carried out. Software using molecular dynamics method has been used to determine the exchange interaction value and monte carlo method has been used to calculate the curie temperature value based on the susceptibility and magnetisation values in $Ni_{10}Fe_{90}$ to $Ni_{90}Fe_{10}$ composition variations. The relationship between the composition variation and the curie temperature value is that the higher the Ni composition will cause the curie temperature value to decrease. The decrease in curie temperature value is caused by the magnetic moment in Fe material is greater than Ni which causes the weakening of interaction so that thermal energy is easier to scramble the spin. The hysteresis curve is used to find an easy axis for magnetised materials, namely the z-axis with a coercivity field of 0.5T. In addition, the relationship between temperature and the shape of the hysteresis curve to identify

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magnetic properties is that the higher the temperature used will cause the value of the coercivity field and remanent magnetisation to be small. Conversely, magnetic saturation will remain at all temperature variations used. This phenomenon is very relevant to the development of material-based technologies such as the manufacture of Hard Disk Drive (HDD) to maximise the performance and stability of the device under certain conditions.

Acknowledgements

We would like to express our gratitude to the computational physics laboratory at the University of Jember for providing facilities and support during the research process. The authors would also like to thank all parties who provided support and guidance during the writing process, enabling the completion of this article.

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