https://doi.org/10.22306/atec.v10i4.214 *Received: 03 July 2024; Revised: 20 Sep. 2024; Accepted: 10 Nov. 2024*

Study of iron-based composite materials using modelling and simulation

Justin Adamko
Institute of Manufacturing Management, Faculty of Manufacturing Technologies, Technical University of Košice, Bayerova 1, 08001 Prešov, Slovak Republic, EU, justin.adamko@tuke.sk (corresponding author)
Livia Provazkova
Institute of Manufacturing Management, Faculty of Manufacturing Technologies, Technical University of Košice, Bayerova 1, 08001 Prešov, Slovak Republic, EU, livia.provazkova@tuke.sk
Denisa Oleksakova
Institute of Manufacturing Management, Faculty of Manufacturing Technologies, Technical University of Košice, Bayerova 1, 08001 Prešov, Slovak Republic, EU, denisa.oleksakova@tuke.sk

Keywords: Hysteresis, composite materials, soft magnetic materials, modelling.

Abstract: Composite materials are materials composed of two or more components that have different physical and chemical properties. These properties complement each other to create a material with unique properties that cannot be achieved by using the individual components alone. Modelling the effect of preparation processes on the properties of composite materials is an important tool to predict the properties of a material prior to its manufacture. This can help in optimizing the preparation technology and obtaining the desired material properties. In the present work the topicality of the problem of iron-based composite materials and the possibilities of modelling and simulation of selected models are presented.

1 Introduction

Magnetic materials are an important part of our lives. Nowadays, these materials have a wide range of application in our homes, cars as well as biomedical needs. Composite magnetic materials are modern magnetic materials. They have been created by combining existing simple materials and the knowledge of physical metallurgy. The base material - the matrix - has the function of a binder. The second component, which includes fibres or dispersed particles, has a reinforcing effect. By composite material we mean substances which are artificially formed, consist of at least two chemically distinct components and the resulting properties of the composites are different from those of the components. Iron-based composite materials are composite materials which contain iron as the main component. These materials are developed by combining iron with other elements or compounds to achieve the desired properties.

There are several approaches to model the influence of technological processes on the properties of composites. One of them is the use of physical models and simulations that include various physical processes such as heat treatment, mechanical stresses, diffusion and interactions between material phases. These models can be based on mathematical equations, numerical methods or engineering simulation software.

Another approach is experimental modelling where the properties of composite materials are investigated under different process settings. This provides experimental data from which relationships and trends between process parameters and material properties can be identified [1].

2 Magnetic materials

Nowadays, magnetic materials have an important position in the economy. These materials can have different physical and magnetic properties according to the arrangement of the fundamental magnetic moments of the atoms of which they are composed. A distinction is made between diamagnetic, paramagnetic and ferromagnetic materials [2].

Magnetic materials are of great importance in engineering and technical practice. Their use has led to a revolution in materials research, physics, electronics and electrical engineering. These materials and their products are used in the design of magnetic circuits, generators, transformers, electric motors, coils, sensors and as storage media in IT technologies. Some magnetic materials have been known for many years while others have only recently been discovered. With the expected advances in the discovery of new magnetic materials their widespread use in areas where they have not yet been applied can be foreseen. Physicists and engineers use electromagnetism in the production of magnetic materials because everything in our environment starting from fundamental particles to groups of galaxies has different electromagnetic properties. In terms of the size of the coercive field, engineering magnetic materials are divided into two basic groups:

1. Magnetically soft materials for which the coercive field value $HC < 100\ Am^{-1}$,
2. Magnetically hard materials where the coercive field HC is greater than 1000 Am^{-1} [3].

2.1 Magnetic soft materials

The term refers to materials that are easily magnetized and can be magnetized repeatedly, and even if the magnetic field is removed, the magnetism disappears. The characteristic feature of this type of material is its high magnetic permeability, Consequently, they can be easily magnetized in a magnetic field and quickly achieve a high magnetization intensity. This type of materials is widely used in high-frequency technologies such as magnetic cores, magnetic heads and memory magnetic cores. Commonly used soft magnets are iron-silicon alloys, iron-nickel alloys and amorphous metals [3].

Magnetically responsive soft materials consisting of ferromagnetic particles and polymer matrix have recently attracted significant research interests due to their untethered, reversible and fast activation under external magnetic fields. The activation and performance of magnetically responsive soft materials largely depend on the magnetization of ferromagnetic particles and structure.

Depending on the magnetization characteristics, ferromagnetic materials can be categorized into soft magnetic materials and hard magnetic materials.

Soft magnetic materials can be easily demagnetized and remagnetized at a relatively small magnetic field. As a result, magnetically sensitive soft materials in which soft magnetic particles are embedded (e.g. magnetorheological elastomers and ferrogels) are usually subjected to simple elongation or shortening deformations by taking advantage of the magnetic force generated in the magnetic field. This limits to some extent the potential of magnetically sensitive soft materials in applications that require complex transformations [3].

Magnetically soft compact powder materials are progressive materials with a rapidly growing application area. They are ferromagnetic materials containing a non-magnetic component in which magnetically soft powder particles are randomly arranged with each other, forming a heterogeneous structure. Depending on their preparation, they can be determined as the so-called compacts (pressed ferromagnetic powder without the addition of insulation) or soft magnetic composites (SMCs), in which the ferromagnetic powder particles are coated with a thin layer of insulation before being pressed [4,5].

In general, magnetically soft materials are used as transformer cores, but they also find applications in motors, inductors and generators. Soft magnetic composite (SMC) material is actually made up of surface-insulated iron powder particles and has a number of advantages including isotropic magnetic and thermal properties, low eddy current losses, and relatively low overall core losses at medium and higher frequencies, but also with the prospect of low-cost mass production. The SMC material, due to its powdery nature and isotropic magnetic properties, is suitable for the construction of electrical machines of three-dimensional (3D) magnetic fluxes and complex structures for which it is almost impossible or very difficult to use layered steels [6].

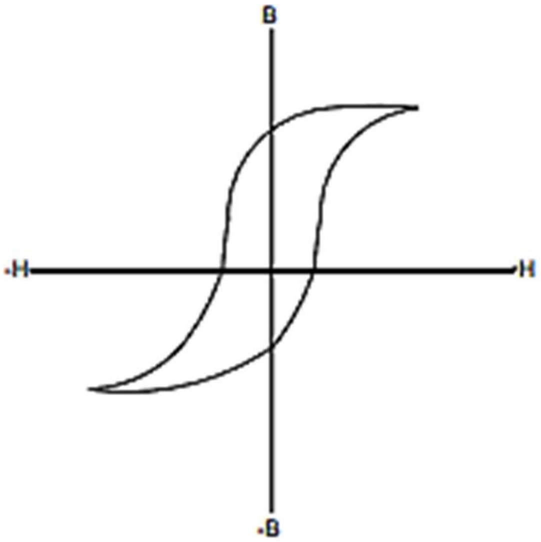

Figure 1 Hysteresis loop of magnetic material

The most important parameters that are determined from the hysteresis loop are the saturation magnetization MS or magnetic induction BS (magnetic flux density), the coercive field HC (the value of the magnetic field strength at which the substance (magnetic) has zero magnetic induction) and the remanent magnetization MR or magnetic induction BR (representing the magnetic induction that remains in the material after the external magnetic field has been switched off). Other important parameters that can be determined from hysteresis loop measurements include the initial permeability µpoc and the maximum permeability µmax (the maximum slope of the B versus H dependence), which can be found in the initial magnetization process. Magnetic induction, referred to as B, is a physical quantity that describes the strength of a magnetic field. It is one of the key parameters in magnetism and plays an important role in the characterization of magnetic fields in various materials. Magnetic induction is correlated with the magnetic field strength (H) and the magnetic permeability of a material. Magnetic induction is used to describe the behavior of magnetic materials as well as to design and analyze electromagnetic devices such as transformers, electric motors, generators, and magnets. In cyclic magnetization of a material, the relationship between B and H is shown in the form of a hysteresis loop, which illustrates the nonlinear and dependent nature of the magnetization of the material, including the energy losses during the cycle. Magnetic induction is a fundamental element in the study of magnetic fields and their interaction with materials, which is important for various applications in industry, technology and science [7-9].

3 Modelling the impact of technological processes

Modelling the influence of technological processes on the properties of composite materials is an important tool in optimising their preparation. In this way, it is possible to predict and analyse how different factors and process parameters affect the properties of materials and their resulting properties. There are several approaches to model the influence of technological processes on the properties of composites. One of them is the use of physical models and simulations that include different physical processes such as heat treatment, mechanical stresses, diffusion and interactions between material phases. These models can be based on mathematical equations, numerical methods or engineering simulation software.

Scientists have been trying to explain and describe ferromagnetic hysteresis for more than 80 years. Over the decades, several approaches have been developed. Micromagnetic methods are used to determine the minimum energy of a system to find the orientation of magnetic moments. These methods are limited to a small range. The other extreme is to fit a measured curve without a physical background. An intermediate solution - a global estimate of the magnetic behaviour based on statistical physics methods modulated by certain microstructural assumptions lies between these two approaches [10,11].

In the second half of the 1980s, another model was proposed by Jiles and Atherton based on Weiss's original ideas on magnetic domains and the effective magnetic field inside a ferromagnetic material, and using a key concept, anhysteretic magnetization, based on a modified Langevin function. Later, Harrison introduced a slightly different concept of ferromagnetic hysteresis with a new dimensionless quantity called the domain coefficient [12,13].

In previous models, the influence of the effective magnetic field is included twice in the energy density equation. This corresponds to the interaction of the magnetic moment with itself. In addition, the flexibility of the domain wall was described by the parameter c, although this parameter was not explicitly defined. These inconsistencies led to the proposal of another differential isotropic model of ferromagnetic hysteresis (DIMFH). In this model, the transition from the paramagnetic Langevin function to the ferromagnetic Langevin function is achieved through the assumption of a magnetic cluster. The fuzzy interaction coefficient α is replaced by a defined interaction coefficient β. The double effective field effect is removed leading to a more stable solution of the model equation, and the coefficient β acquires a different meaning. It turns out that the fixed and flexible interleaving of the attachment sites is indistinguishable for DIMFH (and should be even for previous models) from the interleaving of large curves [12,13].

There are several approaches to ferromagnetic hysteresis loops modelling. Some modelling approaches are based on curve fitting that ignore the fundamental physical properties of the material. On the other hand, other methods take into account all known properties and have a rigorous physical basis but they are too time consuming to be useful for macroscopic applications to real engineering materials. Each value in the modelling of magnetization curves is associated with an infinite number of potential magnetizations depending on the history of the samples [10].

Hysteresis can be caused by three specific phenomena: inter-domain interaction, anisotropy and internal friction. The dominant cause varies from material to material; therefore, it is essential to compare hysteresis in the various models available, which include models such as Stoner - Wolhfarth (S - W), Jiles - Atherton (J - A), Globus and Preisach [12].

Table 1 Comparison of the selected models and their characteristics [15]

Model Characteristics	**Stoner – Wolhfarth**	**Jiles – Atherton**	**Globus**	**Preisachov**
Mechanism	Rotation	Not specified	Wall movement	Not specified
Anisotropy	Uniaxial	Multiaxial	Multiaxial	Not specified
Interaction	Yes	Yes	No	Moving model
Pinning effect	Yes	Yes	Yes	Moving model
Structure	Anisotropic or isotropic	Isotropic	Uniaxial (180 °)	Not specified
Wall energy	No	No	Yes	Yes
Revesibility	Yes	Additional model	Yes	Additional model
Side loops	Yes	-	-	Yes
Demagnetization	-	Yes	-	Yes
Anhysteresis	Yes	Yes	Yes	Yes
Grains	Single domain	Multiple domains	Dual domain	Not specified
Material	Magnetic hard materials	Bulk materials	Soft ferrites	Magnetic thin material

To define the limitations of the use of the available baseline model, the main characteristics and features are summarised in Table 1.

This table shows the importance of the anhysteretic curve, which is defined as the location of global equilibrium states observed in each of the models. It is also clear that a universal model, which is suitable for all kinds of materials, does not yet exist. However, the table allows to highlight similarities and common concepts especially for the J-A, S-W and Globus models, which are physically based models [10].

Based on experimental measurements of coercivity, remanence and saturation magnetization, it is possible to calculate the various model parameters needed to describe hysteresis based on Jiles - Atherton theory, initial anhysteretic susceptibility and maximum deferential susceptibility. The aim is to show the possibilities of determining the hysteresis parameters of experimental hysteresis measurements and then using them to model hysteresis curves. This represents a new development in ferromagnetic hysteresis modelling that allows for the first time to calculate parameters from a set of experimental data. The described method enables to determine the values of these parameters and to an accuracy of a few percent. Comparison of measured and modeled hysteresis loops demonstrates excellent agreement between measured and modeled curves [14].

Accurate modelling of electromagnetic systems is crucial for the development of innovative applications. The micromagnetics approach combines theoretical knowledge with experimental data and plays an important role in this process. For electromagnetic applications, sophisticated modelling techniques need to be developed. Micromagnetic simulation of magnetization dynamics relies on the solution of the nonlinear Landau-Lifshitz-Gilbert (LLG) equation. To simplify the calculations, linearization within the small-angle approximation is commonly used. Interchangeable spring magnets combine hard and soft phase materials to achieve high coercivity, saturation and remanence. They have received considerable attention in the last two decades. The theoretical maximum energy density of the product is given to be around 120 MGOe(mega-gauss-oersted) [14].

The object-oriented micromagnetic framework (OOMMF) was first introduced in 1998. The C++ language is used to write this software. Some commercial software tools allow simulation with finite temperature values. The solution space is divided into rectangular prisms with equal dimensions. In this simulation, A is considered as the exchange constant and M as the magnetization. The total energy in each cell is calculated taking into account the exchange energy, the energy of intrinsic static magnetization, the energy of magnetocrystalline anisotropy as well as the Zeeman energy(or external field energy is the potential energy of a magnetized body in an external magnetic field.). Experimental results show that the remanence is close to the expected values, but the coercivity differs significantly from them. Micromagnetic simulation using 3D OOMMF software allows to reveal the underlying physical phenomena and the influence of the soft phase on the coercivity of nanocomposite magnets.

This study highlights the importance of the microstructure of nanocomposite magnets for understanding their magnetic properties. In addition to high spontaneous magnetization and energy anisotropy, the microstructure plays a key role in the coercivity, remanence and energy density of the product. Micromagnetic simulations allow us to investigate the influence of microstructure on these properties. The theoretical insights from this study can be applied to optimize the properties of nanocomposite magnets. They can be used to select the appropriate soft phase size in the preparation of bulk nanocomposite magnets. Applying numerical methods and computer software, the BH loop of these magnets can be easily calculated, and their performance can be predicted. Micromagnetic simulations also open the way to the development of permanent magnets with low rare-earth content even without omitting them altogether. Simulations will help us to explore the properties of these materials and design optimal compositions for different applications [14].

4 Conclusions

The conclusion shows that despite the popularity of the Jiles-Atherton model of magnetic hysteresis for the treatment of anhysteretic magnetization curves, this model faces challenges in numerical processing that often leads to biased and unreliable results. This can be a hindrance in achieving the objectives effectively using the available software.

On the other hand, modelling the effect of preparation processes on the properties of composite materials has been shown to be a key tool for predicting material properties prior to manufacturing, which helps in optimising the preparation technology. Although this approach offers significant advantages such as accurate prediction of material properties, it is often computationally intensive and does not always provide accurate results.

It is clear that there is currently a lack of simulations that efficiently handle hysteresis loops based on the Jiles-Atherton model, presenting an opportunity for further research and development in this area.

Acknowledgement

This work was funded by Scientific Grant Agency of Ministry of Education of Slovak Republic and Slovak Academy of Science grant numbers VEGA 1/0403/23 and VEGA 1/0016/24.

References

[1] PLUHAR, J., BENEŠ, V.: *Construction and tooling materials*, Praha: ES CVUT, 1980.

[2] DOBRZAŃSKI, L.A., DRAK, M.: Hard magnetic composite materials Nd-Fe-B with additions of iron and X2CrNiMo-17-12-2 steel, *Journal of Alloys and Compounds*, Vol. 449, No. 1-2, pp. 88-92, 2008. https://doi.org/10.1016/j.jallcom.2006.02.092

[3] LU, L., SIM, J., ZHAO, R.R.: Mechanics of hard-magnetic soft materials: A review, *Mechanics of Materials*, Vol. 189, No. February, 104874, 2024. https://doi.org/10.1016/j.mechmat.2023.104874

[4] PÉRIGO, E.A., WEIDENFELLER, B., KOLLÁR, P., FUZER, J.: Past, present and future of soft magnetic composites, *Applied Physics Reviews*, Vol. 5, No. 3, 031301, 2018. https://doi.org/10.1063/1.5027045

[5] Coercive field, [Online], Available: https://beliana.sav.sk/heslo/koercitivne-pole [10 Jun 2024], 2017. (Original in Slovak)

[6] Magnetic materials, [Online], Available: https://www.poziadavka.sk/katalogy/www.poziadavka.sk_4366_56496.pdf [10 Jun 2024], 2007. (Original in Slovak)

[7] Materials with magnetic properties, [Online], Available: https://crushtymks.com/sk/energy-and-power/349-materials-with-magnetic-properties.html [10 Jun 2024], 2019. (Original in Slovak)

[8] ASARI, A., GUO, Y., ZHU, J.: Magnetic properties measurement of soft magnetic composite material (SOMALOY 700) by using 3-D tester, *AIP Conference Proceedings*, Vol. 1875, No. 1, p. 030015, 2017. https://doi.org/10.1063/1.4998386

[9] LIU, CH., LU, J., WANG, Y., LEI, G., ZHU, J., GUO, Y.: Design Issues for claw pole machines with soft magnetic composite cores, *Energies*, Vol. 11, No. 8, 1998, pp. 1-15, 2018. https://doi.org/10.3390/en11081998

[10] LIORZOU, F., PHELPS, B., ATHERTON, D.L.: Macroscopic Models of Magnetization, IEEE Transactions on Magnetics, Vol. 36, No. 2, pp. 418-428, 2000. https://doi.org/10.1109/20.825802

[11] JILES, D.C., ATHERTON, D.L.: Erratum Title of paper: Theory of ferromagnetic hysteresis, *Journal of Magnetism and Magnetic Materials*, Vol. 92, No. 2, p. 289, 1990. https://doi.org/10.1016/0304-8853(90)90646-8

[12] JILES, D.C., THOELKE, J.B., DEVINE, M.K.: Numerical determination of hysteresis parameters the modeling of magnetic properties using the theory of ferromagnetic hysteresis, *IEEE Transactions on Magnetics*, Vol. 28, No. 1, pp. 27-35, 2002. https://doi.org/10.1109/20.119813

[13] CARDELLI, E., DELLA TORRE, E., FABA, A.: Analysis of a unit magnetic particle via the DPC model, *IEEE Transactions on Magnetics*, Vol. 45, No. 11, pp. 5192-5195, 2009. https://doi.org/10.1109/TMAG.2009.2031078

[14] SUNDARA MAHALINGAM, S., MANIKANDAN, B.V., AROCKIARAJ, S.: Review - Micromagnetic Simulation Using OOMMF and Experimental Investigations on Nano Composite Magnets, *Journal of Physics: Conference Series*, Vol. 1172, 012070, pp. 1-11, 2019. https://doi.org/10.1088/1742-6596/1172/1/012070

Review process

Single-blind peer review process.