# Chapter 4 Utilization of data science

## Section 1 Current and Future Utilization of Data Science

### 1.1 Data Science and Power Electronics

**Keywords:** artificial intelligence (AI), machine learning (ML)

Data science is a new academic discipline that analyzes real-world data with the aim of revealing the true nature of phenomena. It has a ripple effect on all existing fields by applying useful knowledge and insights drawn from data to solve various real-world problems. Combining techniques from existing academic systems such as statistics, programming, AI, ML, etc., across disciplines to help solve various problems.

AI is a generic term for technologies that attempt to realize intelligent human behavior on computers. At its core, ML refers to a method of constructing models by learning patterns and regularities from data. In the past, "decision rules" were explicitly given by humans in programs, but in machine learning, algorithms themselves discover them using a large amount of data. For example, deep learning (deep learning) used in image recognition and voice assistants is a type of machine learning that automatically extracts and learns complex patterns using multiple layers of artificial neurons (neural networks: NN). This enables AI systems to improve prediction accuracy through trial and error, just like humans do. In other words, AI refers to intelligent processing in general in a broad sense, and ML is a group of AI methods that improve models based on data.

AI/ML technology has made rapid progress in recent years, and its use is spreading in various industrial fields. The power electronics field is no exception, and applications are being explored for automating design, improving control performance, and optimizing maintenance by predicting failures [(1)(2)]. In this section, examples of AI/ML applications in the power electronics field are introduced from the viewpoints of design, magnetic components, control, failure prediction, and design optimization, and finally, future prospects and issues are discussed.

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### 1.2 AI/ML Application in Power Electronics Circuit Design

**Keywords :** circuit design, simulation, design space exploration

The circuit design process for power electronics equipment covers a wide range of processes from requirement definition, topology selection, component value determination, thermal design, and reliability evaluation, and requires iterative trials that rely on the designer's experience. The introduction of AI/ML is now underway to automate and streamline part of this design process [(1)].

One specific example is the use of surrogate models. High-precision circuit simulations and physical model calculations are time-consuming, but the preparation of ML models that mimic their behavior can significantly reduce calculation costs. For example, by using neural networks to approximate the characteristics of circuits and components, output performance and thermal characteristics can be predicted immediately upon input of design parameters. In reference [(2)], a thermal characteristics and degradation prediction model based on feed-forward NNs (FFNNs) was constructed and successfully used to rapidly estimate junction temperature fluctuations and the degree of annual degradation of semiconductor devices from design parameters. This AI-based approximate model reduces the time required for simulation and increases the number of design trials, thereby shortening the design cycle.

In addition, ML has been used to explore the design space. After defining design goals (e.g., loss minimization, efficiency maximization, etc.) and constraints, the problem of searching for optimal topology and part values can often be treated as a problem involving combinatorial explosion. Evolutionary meta-heuristics (evolutionary algorithms) such as genetic algorithms (GA) and particle swarm optimization (PSO) have been used to solve this problem, and AI techniques can be used to evaluate a wide range of design candidates in a data-driven manner without relying on human intuition, potentially finding high-performance design solutions that were previously overlooked. In general, the introduction of AI/ML has been a good step forward in the design process. In general, the introduction of AI/ML is expected to advance automatic evaluation and optimization from the early stages of circuit design, thereby increasing design accuracy while reducing the amount of labor spent on prototyping and testing. This is discussed in detail in Section 2.

However, AI is not the answer to everything, and it is still essential to build on traditional analytical models. Integrating AI into analytical models can provide practical and reliable design support that combines theoretical underpinnings with data-driven strengths, and can achieve innovation in the design cycle while avoiding excessive reliance on black boxes.

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## 1.3 AI/ML application for property prediction and material development of magnetic components

**Keyword:** Magnetic parts, Magnetic materials

AI/ML is also being used for magnetic components such as inductors and transformers, which play an important role in power electronics. The behavior of magnetic materials (e.g., magnetization characteristics and core loss) is nonlinear and strongly frequency-dependent, making it difficult to reproduce them with high accuracy using conventional physical models alone [(1)]. In response to this issue, many studies have been conducted on modeling magnetic material properties by machine learning.

For example, a method has been proposed that uses an auto-encoder type deep learning model to learn magnetic core characteristics (B-H curves and loss characteristics), including the frequency several MHz region and even the saturation region, and reproduce magnetic characteristics with high accuracy under a wide range of conditions [(2)]. Using such a model, the characteristics of magnetic components can be precisely predicted based on actual measurement data, and iron loss and inductance variations can be quickly estimated during design. In fact, some research results have shown that AI is useful for estimating iron loss in high-frequency operation, using appropriately configured deep NNs to model magnetic core loss with high accuracy [(3)].

In addition, the development of magnetic components combining a large-scale database and AI is also making progress. Princeton University has constructed "MagNet," an open database that accumulates experimental data on magnetic materials, and a project is underway to use it for efficient design of magnetic components and high-precision modeling of magnetic material properties. (4) The combination of rich data such as MagNet and deep learning is accelerating the optimization of magnetic component design, which has been difficult to do manually in the past.

Furthermore, in the field of materials research, AI is also being used to search for new magnetic materials (magnet materials). A team at the Ames Laboratory in the U.S. has developed a machine learning model to discover new permanent magnets that do not contain critical materials such as rare earths. The model predicts the Curie temperatures of materials of various compositions and has succeeded in narrowing down promising compositions that retain their magnetic properties at high temperatures [(5)]. The important point here is not simply to search for new materials, but to define the necessary material properties by working backward from the requirements of the final application side, or "exit requirements," and then use AI to efficiently extract candidates that satisfy these conditions. Using AI in this way enables the discovery of high-performance magnetic material candidates more efficiently than conventional material searches that rely on experiments, and is expected to lead to a dramatic improvement in the performance of future inductors and magnets for motors.

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## 1.4 ML application to real-time control (inverter control, motor drives, etc.)

**Keywords:** fuzzy control, reinforcement learning, AI control

AI/ML is also being used to implement sophisticated control algorithms in the field of power electronics control. Advanced control such as switching control of inverters and converters, vector control of motor drives, and Maximum Power Point Tracking (MPPT) control of power conditioners for renewable energy, etc., require specialized knowledge and experience. AI/ML has the potential to extract performance that cannot be achieved manually by learning these control laws from data and tuning them with optimization methods.

An early application is fuzzy control. Fuzzy inference is an AI method that incorporates expert knowledge into "If-Then" style rules to achieve stable control even when there is some uncertainty. Fuzzy control has long been used in the field of power electronics, and many examples of its application to motor speed control and MPPT control of photovoltaic power generation have been reported [(1)]. Although fuzzy control can operate robustly even in highly nonlinear systems, it requires expertise in rule design, and in recent years, there has been a shift to neural network control and reinforcement learning control.

The advantage of NN-based control law is that it can learn the optimal control function from input and output data even if the exact mathematical model of the system is unknown. This is said to improve adaptability. For example, a study has been reported in which sliding mode control characteristics were learned by NNs to reduce the chattering phenomenon [(2)]. Automatic PID gain adjustment by a GA has also been used to obtain the fastest response, which is difficult to achieve with manual adjustment [(3)]. These are examples of solving these problems by using meta-heuristics, in which the adjustment of control parameters is regarded as an optimization problem.

Meanwhile, the use of reinforcement learning (RL) is also attracting attention as the latest trend in the control field. Reinforcement learning is a method that autonomously learns measures to maximize "rewards" through trial and error, and since it does not require pre-prepared training data, it can acquire optimal control laws in real-time while interacting with the environment. For example, Q-learning RL has been applied to MPPT control of a wind power generation system to maximize power generation sequentially in response to wind fluctuations. [(4)] RL has strengths in optimization under dynamically changing conditions and is expected to be applied to highly efficient operation of motor drives and cooperative control of multi-converter systems in the future. (4) In the future, RL is expected to be applied to highly efficient operation of motor drives and cooperative control of multiple converter systems.

As a concrete example of the effectiveness of these AI controls, results of control optimization using meta-heuristics have been reported. For example, it has been shown that the application of Ant-Colony Optimization (ACO) to a solar MPPT problem under partial shading, which tends to local maxima, improves global convergence and robustness to shading patterns [(5)]. It has also been reported that using the Immune Algorithm (IA) for PWM waveform optimization of single-phase inverters achieves low harmonic distortion (THD 0.79%), which compares favorably with hysteresis control (THD 1.23%) [(6)]. These are examples of AI algorithm-based control showing better performance and tuning efficiency than conventional methods. On the other hand, however, there are issues such as real-time arithmetic processing and stability assurance of control, and careful verification and hardware implementation are required for industrial applications.

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## 1.5 Application of AI/ML for failure prediction and anomaly detection

**Keyword:** Aging, Predictive maintenance, Usable life

AI/ML is also being used in the fields of failure prediction and abnormality detection to highly improve the reliability of power electronics systems. Capacitors and semiconductor devices in power electronics equipment deteriorate over time, causing performance degradation. If AI/ML can detect the signs of such deterioration early using sensor data, planned parts replacement can prevent unexpected downtime. Recently, there has been a movement to introduce predictive maintenance in energy infrastructure and manufacturing equipment, where AI/ML has begun to predict long-term degradation and test equipment under various scenarios (1).

Approaches to anomaly detection can be broadly divided into supervised and unsupervised learning. In the supervised approach, a normal/abnormal classifier (e.g., NN or support vector machine (SVM)) is trained using past fault data to automatically discriminate fault modes for new data. For example, there is an attempt to detect abnormalities in rectifier circuits by constructing an FFNN that takes input voltage/current and output current as inputs and estimates output voltage (2). This is a method in which the NN learns the normal input-output relationship and considers an abnormality if the error with the measured output exceeds a threshold value, thus detecting signs of abnormality from sensor data in the same manner as a skilled human operator.

On the other hand, unsupervised learning (anomaly detection) is effective when sufficient failure data is not available. This method learns only normal data and considers any deviation from normal as an anomaly, using clustering (k-means), self-organizing maps (SOM), and Isolation Forest. For example, an anomaly detection model "ResFaultyMan" using the Isolation Forest algorithm has been proposed and shown to be adaptable to various failure scenarios (3). This model effectively isolates outliers (abnormal behavior) through its tree structure and can detect abnormalities in power electronics equipment with higher accuracy than One-Class SVM or local outlier factor methods.

In failure prediction, research is also underway to estimate the remaining useful life (RUL) from the current degradation state. For example, a method combining Gray-Wolf optimization and support vector regression (SVR) has been reported to predict the RUL of DC-DC converters (4). This statistical data-driven method can predict the transition of degradation indicators such as capacitor capacitance degradation and semiconductor on-resistance increase, and can quantitatively estimate the time to failure. The prediction results can be utilized to optimize maintenance planning, enabling predictive maintenance in which necessary parts are replaced when needed (1).

In the industrial world, some advanced power electronics products are already incorporating self-diagnosis and predictive detection functions. For example, in large-scale renewable energy facilities and industrial inverters, data from temperature, vibration, and current sensors are being collected in the cloud, and machine learning models are being used to analyze degradation. PHM (Prognostics and Health Management) technology is developing in line with the IEEE standard framework (5) and is expected to become a key technology for improving reliability in the power electronics field in the future.

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## 1.6 AI/ML application to topology selection and parameter optimization

**Keywords:** topology selection, multi-objective optimization, Pareto solution

AI/ML is also gaining attention as a promising solution in the area of power electronics circuit topology selection and parameter optimization. AI/ML has been proposed to automate this process and search for the optimum solution.

As an example of the latest research, the "ML-ACCEPT" system developed by a group at the University of Michigan and others shows a framework that uses ML to automatically recommend a DC-DC converter circuit scheme class suitable for a given specification, and then combines RL and deep NN to optimize the final element values (1). This system uses a hybrid of multiple AI techniques to suggest the optimal topology and design parameters with high accuracy from the designer's input. The innovation is that initial circuit selection, which previously relied on the experience and guidance of experts, can be automated in a data-driven manner.

Another method uses a surrogate model with deep learning to predict performance indices for various topologies and attempts to select the most efficient converter method (2). In this paper, DNN models are trained individually using a large amount of simulation data for typical

DC/AC converters, so that the predicted efficiency of each topology can be immediately output from the input specifications. A reinforcement learning agent then evaluates the DNN predictions and performs a search to quickly determine the optimal method without additional large-scale simulations. This approach dramatically reduces the time required to compare multiple topologies.

AI/ML is also used for multi-objective optimization of power electronics design. For example, when simultaneously optimizing multiple goals such as efficiency, cost, and weight of a power converter, it is necessary to find a set of Pareto-optimal solutions. For this problem, a type of genetic algorithm, such as non-superior sorting GA (NSGA-II), is often used. In reference (3), NSGA-II was successfully applied to the design optimization of an IGBT power module to obtain an optimal design set that takes into account thermal and lifetime characteristics. Although such evolutionary methods are optimization algorithms rather than AI, they are positioned as AI technologies in a broad sense and have been actively used in recent years, including improved versions of GA and PSO. Furthermore, some studies have emerged with a view to automatically generating discrete topologies by combining them with deep learning and reinforcement learning (4).

As described above, AI/ML is permeating the entire power electronics design optimization process. Data-driven automatic optimization in various steps, from topology selection to component value calculation, layout optimization (wiring pattern optimization), and thermal design, directly leads to significant reductions in design time and cost.


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## 1.7 Future Research Trends and Technical Issues and Prospects

**Keywords:** topology selection, multi-objective optimization, Pareto solution

In the full-scale introduction of AI/ML in the power electronics field, several technical issues and challenging problems to be overcome have been pointed out (1). First is the issue of computational cost. Deep learning and evolutionary algorithms require high computational costs, and it is difficult to directly apply them to power electronics control, which operates with control cycles on the order of microseconds. In the future, it will be essential to develop real-time implementation technologies such as FPGAs, dedicated AI accelerators, and model lightening (distillation and quantization). Second, there is the problem of not having enough training data. In particular, there are many cases where rare failure data is not sufficient for failure prediction, and data augmentation through simulation and data expansion is required. An approach such as training AI by generating virtual data with digital twin technology is also promising and should be deeply considered (2). Third is to address implementation constraints. The third issue is how to deal with implementation restrictions. Another important theme is to increase the explainability (XAI) of deep learning, which is a black box model, and to gain engineers' understanding and trust in the prediction results. In this sense, analytical models remain important, and integration of analytical models and AI is a promising direction.

In light of these issues, several future trends are expected. One of them is the fusion of different fields and total optimization. By combining expertise in the power electronics field (domain knowledge) with knowledge in the AI field, we can expect to see the development of physically informed AI that learns in a manner that does not violate the laws of physics, and optimization algorithms that take into account constraints. In fact, researchers in power engineering and data science are increasingly collaborating, and hybrid methods integrating advanced model-based control and machine learning are expected to develop. Furthermore, for example, a surrogate model that derives characteristics from the physical parameters of magnetic elements can be propagated in the reverse direction to predict the physical parameters to satisfy the exit requirements. This leads to an "inverse problem" approach to define development goals for magnetic elements.

Another important new direction is the use of large-scale language models (LLMs): in 2024, an attempt to automatically calculate the design parameters of power electronics circuits from given requirements using a generative AI such as GPT was reported (3). In 2025, an interactive design tool was proposed that uses GPT as its core and works with circuit simulators and Python-based optimization programs via APIs. A tool has been proposed that works with circuit simulators and Python-based optimization programs via APIs. In this tool, typical circuit topologies are registered in advance, and topology selection and optimization control are realized through natural language dialogue with the designer. In addition, the objective function can be flexibly set in the dialogue, so that LLM functions as an advanced user interface instead of a conventional GUI (4). Thus, a future in which LLMs with learned expertise act as designers' assistants and automatically generate draft schematics and control laws from specifications is not so far off.

Finally, we will discuss the development of AI for industrial applications. In areas where large numbers of power electronics devices are installed in the real world, such as renewable energy systems, power electronics equipment for electric vehicles, and data center power supplies, AI-based efficiency optimization operations and predictive maintenance services will expand as a business. For example, in the smart grid, each power converter is connected by IoT, and cloud AI will optimize supply and demand forecasting and equipment control. This will contribute to more efficient and stable energy use, and should also contribute to the realization of a carbon-neutral society.

The application of AI/ML to the power electronics field has great potential throughout the entire lifecycle of design, control, and maintenance. Although many technologies are still in the research stage, breakthroughs in both academic research and industrial applications are expected to accelerate with the development of fundamental data and advances in computational resources. As the integration of AI and power electronics deepens while addressing future issues, new developments are expected toward the realization of more efficient and reliable power electronics systems.

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# Section 2 Application of AI/ML to Power Electronics Circuit Design

## 2.1 Circuit design problem description from an AI/ML perspective

**Keywords:** circuit model, evaluation function, optimal circuit design, differential equation solver, heuristic optimization

In general, a power electronics circuit is represented $\dot{x} = f(x, \theta, \lambda)$, in steady state by where $x$ is the state variable of the circuit, θ=ωt is the angular displacement, and λ is the circuit parameter. Furthermore, the conditions of power electronics circuits are often discussed in the steady state, and we can say that time θ is in the steady state if $x(\theta) = x(\theta + 2\pi)$ satisfies at any θ. Under this definition, most of the design problems of power electronics circuits can be attributed to the optimization problem of finding a parameter λ that maximizes (or minimizes) the evaluation function $F(x, \theta, \lambda)$. Here, F can include almost anything that can be expressed on a computer, such as output power, power conversion efficiency, switching voltage, and device volume.

In solving this optimization problem, traditional analytical approaches have their limitations, and a computer-based solution search is effective. The necessary software elements are a simulation section to estimate the evaluation function and an optimization algorithm.

## 2.2 Example of AI/ML optimization software configuration

**Keywords:** optimal circuit design, differential equation solver, heuristic optimization

**Figure 4.2.2.1** shows a conceptual diagram of the optimization software. In this unit, the "circuit model description" gives the circuit topology and the circuit equations depending on the devices. For example, nonlinearities of the parasitic capacitance of the output capacitance of a switching device or the forward voltage of a diode can be considered. For example, by preparing a model that relates the geometrical and physical parameters of magnetic elements (core shape, winding diameter, number of turns) to electrical parameters (self-inductance, mutual inductance, equivalent series resistance), it is possible to include magnetic element design parameters in the circuit model.

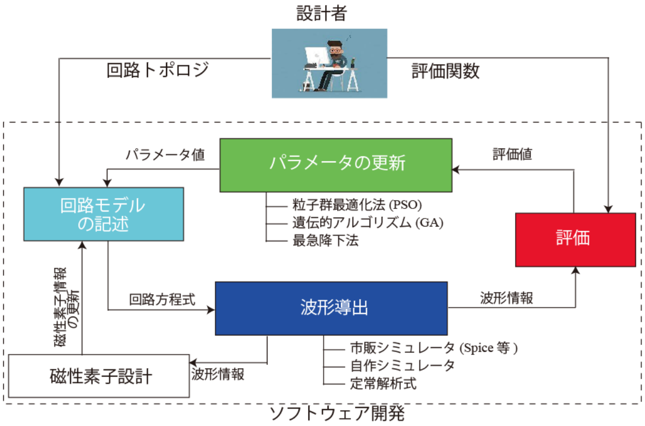


**Figure 4.2.2.1** Software configuration

The "waveform derivation" is a so-called circuit simulator, and it is possible to create your own differential equation solver based on the Eulerian and Runge-Kutta methods, not to mention general-purpose software such as Spice. If voltage/current waveforms based on the circuit model can be derived, various circuit responses can be evaluated. Output power, power conversion efficiency (1), THD (Total Harmonic Distortion) of the AC current, and the fact that the switching device is below the breakdown voltage can also be included as conditions (2).

The circuit parameters are changed according to the obtained evaluation function values, and the optimal parameters are searched for. Since the parameter space is high-dimensional, an efficient solution search is required. For example, heuristic optimization algorithms such as Particle Swarm Optimization (PSO), Genetic Algorithm (GA), and Simulated Annealing (SA) are well known. This updated parameter update is called the "parameter update". This updated parameter update is reflected in the "circuit model description" and the circuit equations are updated. By repeating this loop, the parameters that minimize the evaluation function can be derived, which is synonymous with optimal circuit design.

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## 2.3 Example of optimal design for high-frequency converter

**Keyword:** Class-E$^2$ converter, Switching device model, Magnetic element model

As an illustrative example, an optimal design process for a high-frequency converter is carried out. Specifically, software-based optimization was performed for the Class-E$^2$ converter shown in **Figure 4.2.3.1**. The accuracy of the design depends on the modeling of individual components; for instance, the model for the GaN Systems GS66516 switching device incorporates parameters such as on-resistance, parasitic inductance, and the nonlinearity of parasitic capacitance (Coss). Regarding magnetic components (the isolation transformer $L_1$–$L_2$ and resonant inductor $L_0$), design options—such as core specifications (relative permeability and Steinmetz equation parameters), wire gauge, and number of turns—are prepared and integrated into a mathematical model that calculates self-inductance, mutual inductance, and equivalent series resistance based on these combinations.Regarding the magnetic components (isolation transformer $L_1$–$L_2$ and resonant inductor $L_0$), parameters such as core

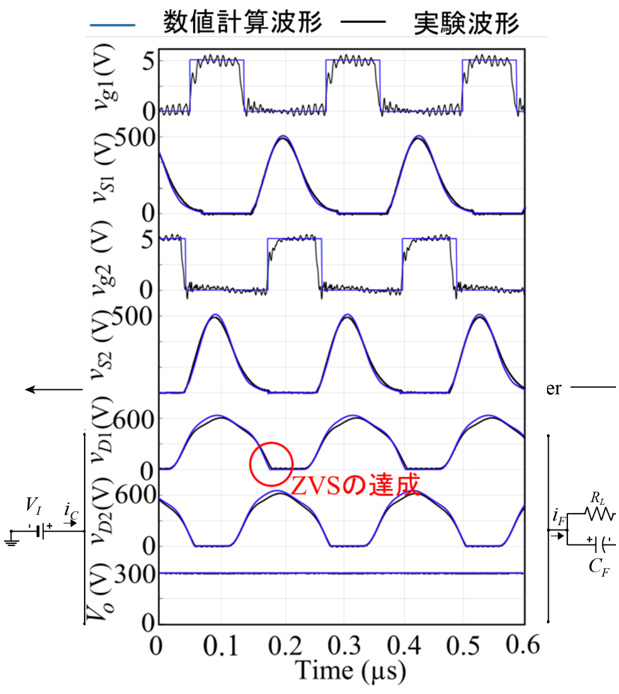


**Figure 4.2.3.2** Operating waveforms of the optimized Class-E$^2$ converter

characteristics (relative permeability and Steinmetz equation coefficients), wire gauge, and number of turns were defined as variables; these were incorporated into a mathematical model that calculates self-inductance, mutual inductance, and equivalent series resistance based on the selected combinations. Using this framework, the software determined the component values that maximize power conversion efficiency for a rated output of 1 kW at an operating frequency of 4 MHz. Figure 4.2.3.2 shows the optimal waveforms derived by the software alongside the corresponding experimental waveforms; the experimental results align closely with the software's predictions. As a result of this optimization aimed at maximizing efficiency, the experiment achieved a power conversion efficiency of 95.3%, setting a record-high figure at the time [1].

From the waveforms in **Figure 4.2.3.2**, it can be seen that the switch waveforms satisfy ZVS. In addition, the optimal solution is presented as the parameter for which the ratio of iron loss to copper loss is almost equal in the isolation transformer and resonant inductor. The software only worked to maximize efficiency. In other words, the optimization software has learned in a very short time the same efficiency maximization technique that we have theoretically considered to be correct, without any special theory (knowledge) being given by humans. This fact fully demonstrates the power and potential of AI in design.

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## 2.4 Expanding AI/ML Design to Inverse Problems

**Keywords:** magnetic element model, inverse problem

In many power electronics circuit designs, circuit design and passive element design are linked but not integrated. There is an inherent interdependence problem in that the electrical parameters of magnetic elements, such as equivalent series resistance, which determines loss, depend on the flowing current, while the current depends on the electrical parameters of the magnetic elements. This problem converges to an equilibrium solution by alternating magnetic element design and circuit experiments. It is a natural idea to repeat this iteration using computer simulation.

On the other hand, the aforementioned optimization can be viewed as deriving the physical and geometric parameters of the magnetic device to realize them, i.e., the type of iron core, winding diameter, number of turns, gap length, etc., from the design specifications and optimization conditions of the circuit design. In other words, if there exists a mathematical model or surrogate model that converts the physical and geometric parameters of the passive device into electrical parameters, then in the reverse direction, that is, given the design conditions of the power electronics circuit, the "ideal" physical parameters of the magnetic device that satisfy those conditions can be given. This is defined as the "inverse problem. The physical parameters presented here suggest the physical parameters of magnetic elements that we "want" to achieve from the standpoint of circuit design. This is expected to lead to the elimination of mismatches between the circuit development and device development directions. On the other hand, whether the physical parameters suggested by the circuit side can be realized as materials in reality is another matter, and feedback from the material side on the calculated parameters is necessary. Repeating this process will lead to constructive discussions between the circuit side and the material side. In other words, AI/ML acts as an intermediary between developers on the circuit side and the material side. This is one of the applications of AI in power electronics circuit design.

[Hiroo Sekiya]

# Section 3 Machine Learning Modeling

## 3.1 Introduction.

**Keyword:** Materials Informatics, Physical model, Extended free energy model

The development of materials informatics has led to dramatic progress in the functional design of materials. In recent years, various research and development activities have been actively conducted on magnetic materials, such as hierarchical connection of structure and function, efficient material exploration, and discovery of hidden information. In particular, a major advantage of materials informatics is that it can lead to new discoveries through data-driven analysis of complex physical properties.

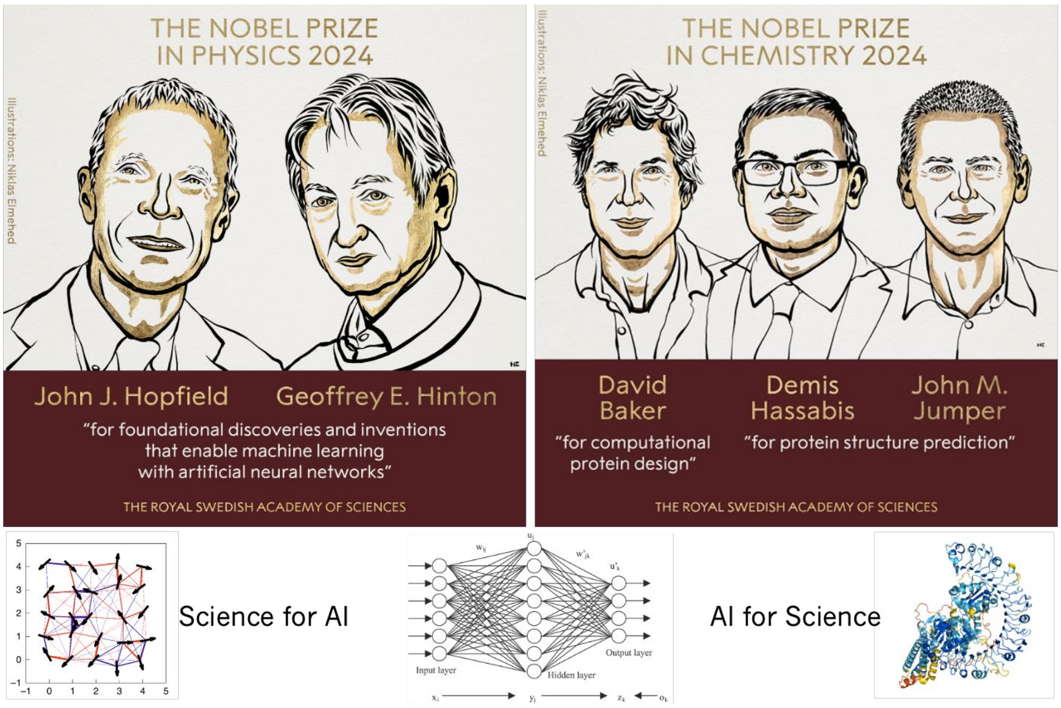


**Figure 4.3.1.1** The 2024 Nobel Prize in Physics and the Nobel Prize in Chemistry. Both were awarded for research results

Functional design of soft magnetic materials for passive components in power electronics is underway to meet the required iron loss and magnetic permeability, but many issues remain to be solved. In particular, the effects of crystal structure and magnetic domain structure on iron loss are extremely complex, and conventional analysis is extremely difficult. Abnormal overcurrent loss is one example. Although the Steinmetz formula can handle fast magnetization reversal, it is difficult to accurately handle spatial inhomogeneity and abnormal vortex loss. Many problems exist behind this, including various approximations and lack of data. In particular, there is a lack of analytical methods for iron loss associated with sudden changes in magnetic domain structure, and a basic understanding of the relationship between the speed of magnetic wall movement and loss energy has not been sufficient. On the other hand, these issues are excellent targets for a data-driven approach to materials informatics.

The Nobel Prize in Physics in 2024 was awarded for his work on magnetic interactions in spin glasses, which led to the construction of an artificial neural network. Furthermore, the Nobel Prize in Chemistry in the same year was awarded for the prediction of protein structure using the artificial neural network. These examples show that data science and magnetic materials science have an inherently high affinity (**Fig. 4.3.1.1**). In this context, the "extended Landau free energy model," which combines magnetic physics and information science, has recently been developed, and progress has been made in analyzing the mechanism of iron loss.

The model analyzes the free energy topography behind the iron loss in data space, allowing the connection of macro-functions and micro-structures across hierarchies. The model is designed in a physics-rooted, white-box fashion, so that the loss mechanisms can be understood and the causes of the functions can be visualized. Advanced analysis and functional design of soft magnetic materials is possible by utilizing large amounts of data and revealing hidden correlations and causal relationships. In this paper, after giving an overview of materials informatics, we will touch on some examples of materials development and describe automated data acquisition techniques. The basic principles of the extended Landau free energy model are then explained, and examples of analyses for various soft magnetic materials are presented. Finally, expectations for power electronics from the viewpoint of materials informatics are also discussed.

## 3.2 Materials Informatics Overview

**Keywords :** Materials Informatics, Measurement Informatics

Materials informatics is a technology that integrates computation and experiment to develop materials with high efficiency and accuracy. Traditionally, computation and experiment have developed independently, but in recent years, there has been an accelerating trend to utilize both of them for materials development (**Fig. 4.3.2.1**). Traditionally, materials development has relied heavily on the expertise, experience, and intuition of researchers. In recent years, however, the amount of research data generated has increased dramatically with the acceleration of calculations and experiments. Therefore, the introduction of data science is expected to systematically extract the essential features inherent in materials and to acquire knowledge that cannot be captured by conventional empirical rules and physical models alone. The scope of this research is not limited to magnetic materials, but extends to batteries, polymers, catalysts, semiconductors, and various other materials.

Next, I would like to introduce several approaches actually used in materials informatics. First, virtual screening is a method that combines computational simulation and machine learning to search for optimal materials from among a huge number of candidate materials, and contributes to the discovery of new materials because it can quickly select promising compositions and structures. Process Informatics analyzes vast amounts of data on manufacturing processes and predicts optimal synthesis conditions and parameters to realize stable production of high-performance materials. Metrology Informatics enhances the feedback loop of development by utilizing measurement data such as magnetic imaging, spectral analysis, and X-ray structural analysis to evaluate the microstructure and properties of materials with high precision. Physics informatics is promising for causal analysis, and physics-based deep learning, such as Physics-Informed Neural Networks (PINNs), has been actively developed in recent years. The extended Landau free energy model introduced in this paper is also a method of physics informatics. In summary, MI (Materials Informatics) is currently being used in the following situations.

**New material exploration**: Integrate computational and experimental data to predict high-performance materials with machine learning models.

**Process optimization**: Optimize the parameters of the manufacturing process to achieve stable production of high-performance materials.

**Experimental design**: Streamline conventional trial-and-error experimental design to quickly find optimal conditions.

**Causal analysis**: A data-driven approach is used to clarify the relationship between physical properties and structure.

Thus, Materials Informatics promotes the integration of computation and experiment and dramatically improves the efficiency and accuracy of materials development. The following is an overview of the materials informatics approach that utilizes computation and experiment.

### 3.2.1 Computational Approach

With the development of computational materials science, first-principles calculations (DFT) and magnetic domain structure calculations (Micromagnetic Simulation) have become widely used. First-principles calculations enable detailed analysis of electronic structures and contribute to the prediction of physical properties such as crystal structures and magnetic anisotropy. On the other hand, magnetic domain


**Figure 4.3.2.1** Overview of Materials Informatics

structure calculations are useful for understanding magnetization dynamics by simulating magnetic wall motion and changes in spin configuration. Materials Informatics utilizes these computational methods to precisely predict the electronic states and magnetic properties of materials and to confirm the consistency with experiments. Furthermore, by combining machine learning such as Bayesian inference, large-scale data can be utilized to accelerate the search for new materials.

#### 3.2.2 Experimental Approach

In the experimental approach, process control of materials and high-throughput measurement techniques are important. In process optimization, precise control of synthesis conditions (temperature, pressure, composition) is required to achieve desired physical properties. In addition, a database of high-precision process parameters enables data-driven control of the manufacturing process, which improves reproducibility and speeds up the search for optimal manufacturing conditions.

Advances in measurement techniques are also important for the development of MI. In particular, measurement techniques such as magnetic imaging, spectral analysis, and X-ray structural analysis have contributed to improving the accuracy of experimental data [(1)]. In magnetic imaging, Kerr microscopy and synchrotron radiation photoelectron emission microscopy (PEEM) enable detailed observation of magnetic domains and visual analysis of spin structures and magnetic wall motion [(2)-(12)]. In spectral analysis, magnetic anisotropy and electron spin state can be quantitatively evaluated by magnetic circular dichroism (XMCD) and spin-resolved angle-resolved photoemission spectroscopy (SARPES) to better understand the magnetic properties of materials [(13)-(14)]. Furthermore, X-ray structural analysis enables detailed evaluation of the correlation between physical properties and structure of magnetic materials through the analysis of crystal structures, and quantitative measurement of the effects of anisotropy and stress. By utilizing such multimodal measurement techniques, multi-scale property analysis becomes possible, and a comprehensive understanding of the relationship between the microscopic crystal structure and magnetic domain structure and the macroscopic iron loss becomes possible.

Large-scale data generated by these technologies can be used for more precise materials design. Thus, materials informatics is an interdisciplinary approach that integrates materials science and data science to streamline materials development and the development process. advances in AI technology and improvements in computation and measurement techniques are bringing innovation to materials development.

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## 3.3 Modeling of magnetic elements and iron loss analysis

**Keyword:** Magnetic domain structure, Magnetic wall, Hysteresis loss

To understand the operating principles of magnetic devices and to design them efficiently, it is essential to analyze the magnetic domain structure and the magnetization reversal process. The magnetic domain structure is a microstructure formed by regions of different magnetization within a magnetic material, and changes in this structure are the key to the iron loss mechanism. In particular, it is known that the movement of the magnetic wall (the boundary where different magnetic domains meet) has a significant effect on magnetic properties and iron loss.

Magnetization reversal is a process in which magnetic domains grow and shrink by the application of an external magnetic field, and it proceeds by the movement and rotation of magnetic walls. Especially in high-frequency environments, the movement of magnetic walls becomes rapid and is the main cause of iron loss. Iron loss is the energy lost by magnetic materials due to changes in the magnetic field, and is mainly composed of three elements: hysteresis loss, eddy current loss, and abnormal overcurrent loss. Hysteresis loss is the energy loss associated with the movement of magnetic walls during magnetization reversal, and depends on the coercivity of the actual material. On the other hand, eddy current loss is caused by the release of energy as heat inside the magnetic material by the current induced by the magnetic field change. Anomalous overcurrent loss is caused by the dynamic behavior of magnetic walls at high frequencies and cannot be adequately described by conventional models. The Steinmetz equation has been widely used in conventional iron loss analysis, but this model assumes the application of a uniform magnetic field, and it has been considered difficult to accurately handle the local effects of magnetic domain structure and abnormal overcurrent loss.

In recent years, data-driven analysis methods have been attracting attention, and more detailed understanding of loss mechanisms is being achieved by directly analyzing magnetic domain structures. In the next section, we describe the extended Landau free energy model developed to overcome these issues and introduce a more precise analysis method for magnetic materials.

## 3.4 Magnetization reversal analysis with extended Landau free energy model

**Keywords:** extended Landau free energy model, persistent homology, energy analysis, visualization

### 3.4.1 Model Overview

The extended Landau free energy model (**Figure 4.3.4.1)** is a method that combines the traditional Landau free energy model with the data science approach to rationally connect the microscopic magnetic domain structure and macroscopic magnetic functions [(1)-(10)]. This model reconfigures the conventional Landau free energy model with the approach of information science to connect the relationship between the microstructure and macroscopic functions in a white-box manner by connecting the change in structure and the change in free energy in the data space. In magnetic materials, the mechanism of pinning phenomenon and iron loss in the magnetization reversal process can be understood in detail, and the polarization point and gradient of the free energy topography can be analyzed in a data-driven manner.

The conventional Landau free energy model describes magnetization reversal as a transition on an energy landscape, but it has the limitation that it cannot sufficiently deal with inhomogeneity of the magnetic domain structure and local pinning phenomena because it assumes perfect crystallinity. In contrast, the present model comprehensively describes the dynamics of magnetization reversal by formulating the magnetic domain structure as a physics-based feature and analyzing the energy landscape in the feature (information) space. In particular, by quantifying the shape and connectivity of magnetic domain structures using persistent homology (PH), a topological method, and by analyzing the correlation between PH and free energy changes, we can clarify the factors governing magnetic wall migration and pinning phenomena. This

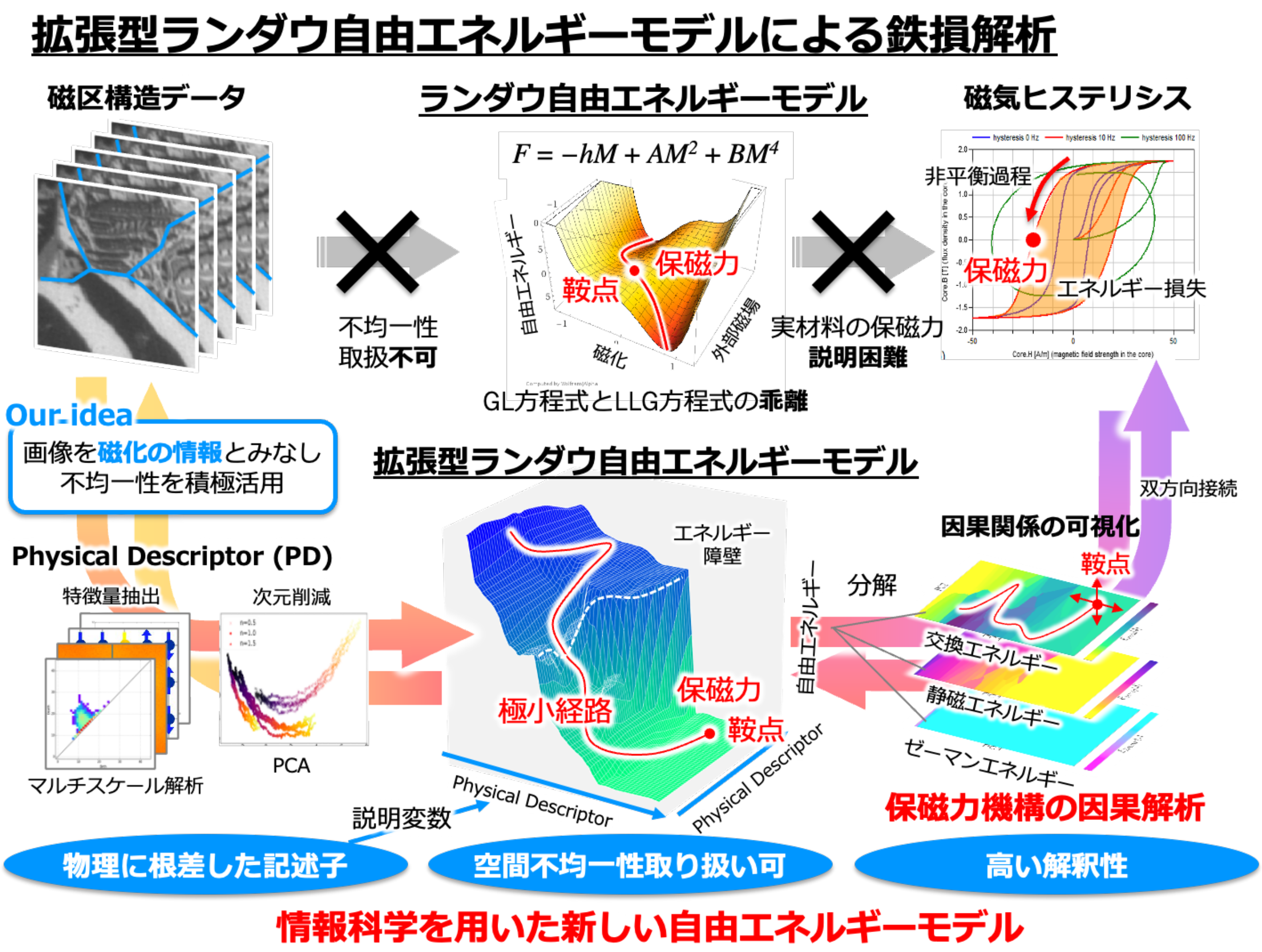


**Figure 4.3.4.1** Overview of the extended free energy model

approach is unique in that it uses interpretable features based on free energy and topology and provides a white-box connection between microstructure and macroscopic functions and their manifestation mechanisms.

Specifically, PH is used to describe the inhomogeneity of the magnetic domain structure, and principal component analysis (PCA) is used to extract changes in the magnetic domain structure as feature vectors (**Figure 4.3.4.2**). By establishing a relationship between the obtained features of the structure and the free energy, we connect the microstructure to the macroscopic features. Furthermore, by analyzing the gradient of the free energy with the features of the structure, the energy barrier is extracted as a multidimensional vector quantity. Using the obtained energy barriers, we can quantitatively evaluate how the microscopic features of the magnetic domain structure affect the energy topography. Furthermore, a component decomposition of the free energy is performed to separate different contributions such as magnetostatic energy and exchange energy. Specifically, each physical role is reconstructed as a PH vector utilizing the Adamar product, which is then visualized back to the original magnetic domain structure. This enables a deep and detailed analysis of the magnetization reversal mechanism. As a result, the structure of energy barriers and factors that promote or inhibit magnetization reversal can be evaluated from the viewpoint of causal analysis. In addition, this model incorporates explainable machine learning, and is characterized by its ability to analyze the microscopic magnetic domain structure and macroscopic magnetic functions while converting between them. This bidirectional analysis enables optimization of magnetic material design based on physical background, rather than mere black-box prediction.

Since this approach is a physics-based white-box model, it easily explains the mechanisms of magnetic wall migration and abnormal overcurrent loss, and achieves higher prediction accuracy than conventional empirical methods. Furthermore, the model can clarify design guidelines for magnetic materials and can be applied to the optimization of materials for power electronics. The features of this model are as follows

**Energy landscape rendering on information space**: Visualize changes in magnetic domain structure as an energy landscape in data space.

**Realization of bi-directional connection**: Integrated analysis of micro magnetic domain structure and macromagnetic function.

**Causal analysis**: Identify the dominant factors of the pinning phenomenon and clarify the relationship with defects and magnetic wall migration.

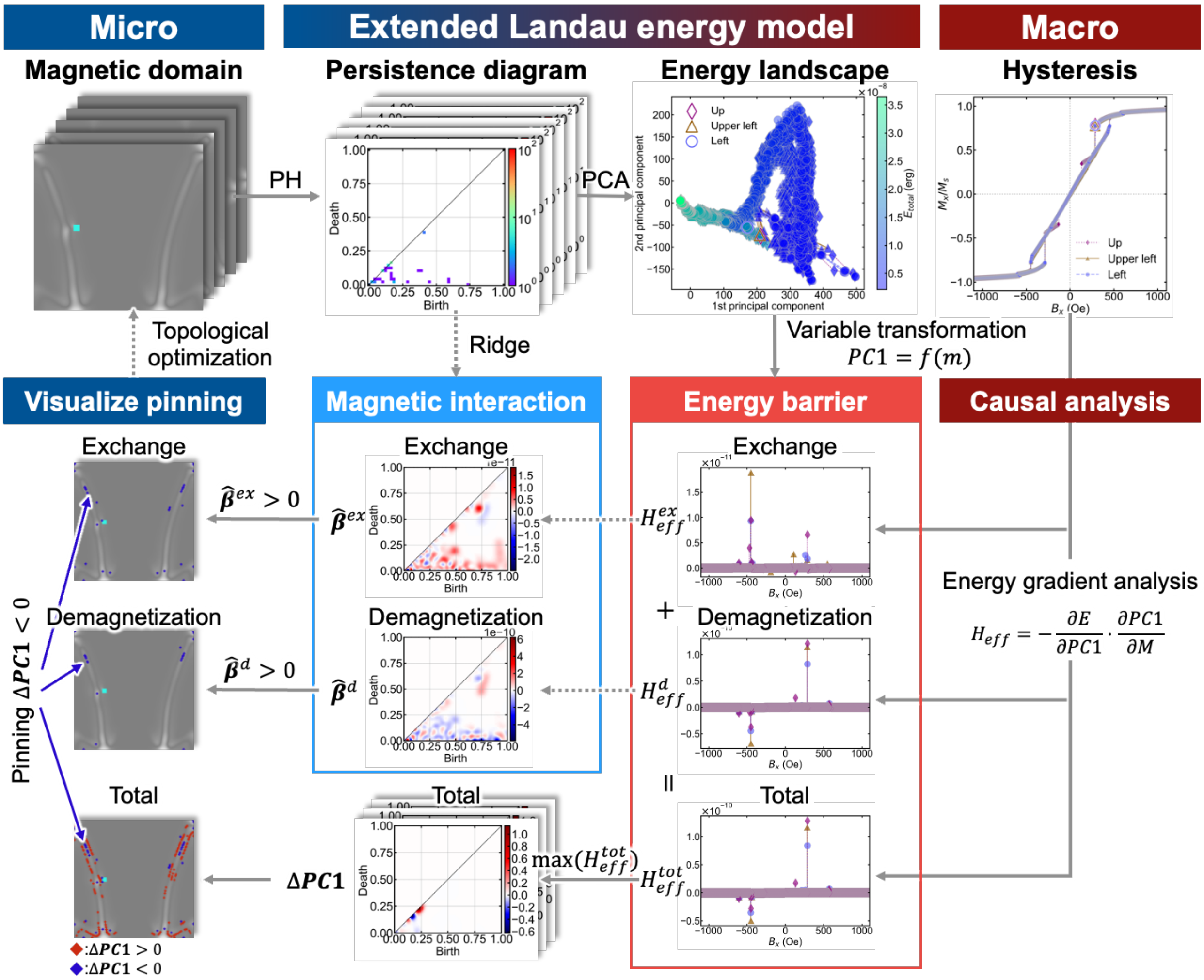


**Figure 4.3.4.2** How to design an extended free energy model

### 3.4.2 modeling technique

**(1) Magnetic domain structure analysis using persistent homology**

With the development of data science, methods of image analysis have evolved greatly in recent years. Traditionally, the physical properties of materials have been evaluated using grain size and other parameters. However, these methods cannot adequately capture complex spatial features and are limited in their ability to provide a detailed understanding of the relationship between structure and physical properties. Therefore, structural analysis based on persistent homology (PH) using topology has been attracting attention in recent years ( **Fig. 4.3.4.3**) [(6)(11)-(16)].

PH is a method for mathematically capturing the geometrical features of data and quantifying the geometric characteristics of magnetic domain structures. Unlike conventional image analysis, PH can describe the geometric features of data as vector quantities. Therefore, the complex structure of magnetic domains can be numerically represented and their changes can be traced.

Specifically, PH binarizes an image by continuously changing its threshold value, recording when a structure appears (birth) and when it disappears in association with others (disappearance). In the figure, starting from an 8-bit grayscale image, grayscale filtration is performed by decreasing the threshold value from the one with the highest luminance. As the threshold is raised, islands of black pixels are born one after another, and eventually they are connected to neighboring islands and disappear. The persistence diagram (PD) shows the luminance of the birth and death of each island as dots, with (a) and (b) corresponding to specific conjunction events. By back-analyzing the corresponding regions on the original image, we can show where the connection occurred and quantify the spatial inhomogeneity (connection and spread) of the magnetic domain structure. As a result, the movement of magnetic walls and the birth and disappearance of magnetic vortices can be described as a persistence diagram, enabling quantitative analysis of changes in the magnetic domain structure. In other words, since changes in the magnetic domain structure have a significant impact on iron loss and magnetization reversal, the birth and disappearance of magnetic domains can be analyzed in detail by utilizing PH.

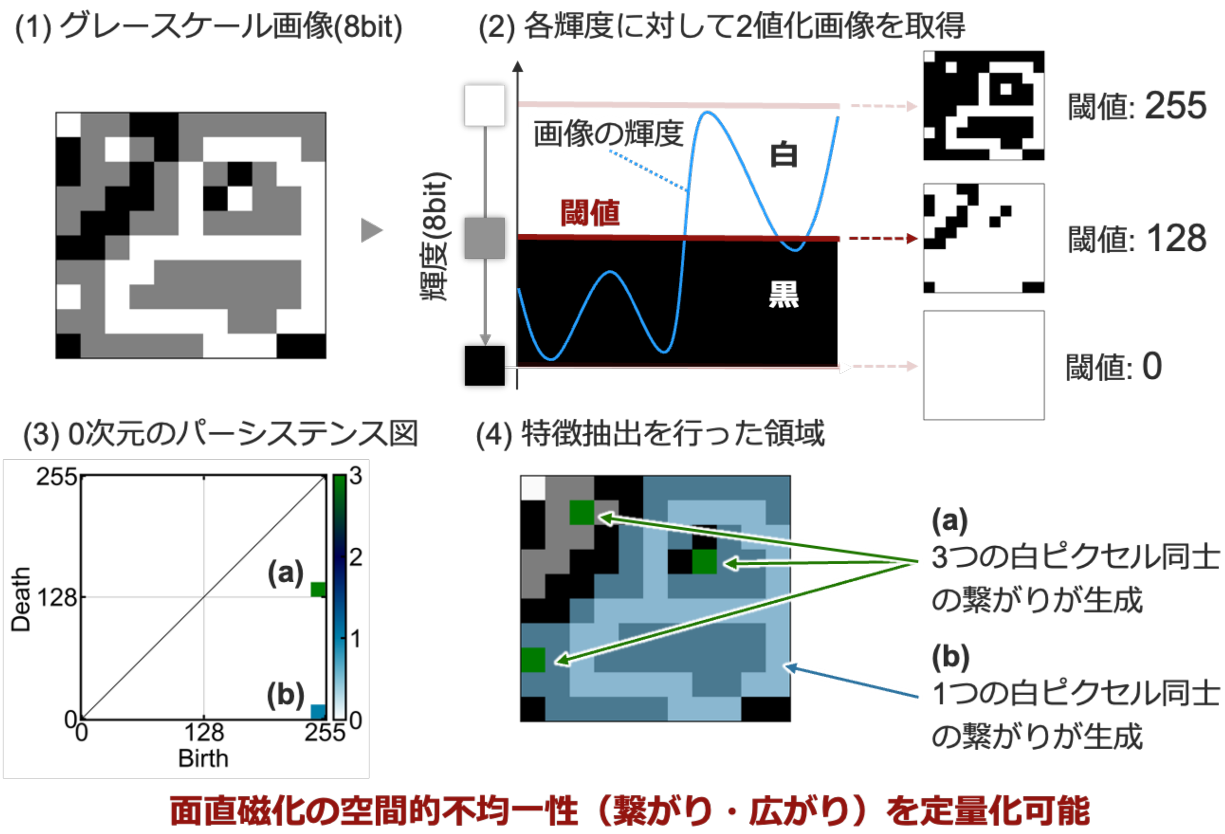


**Figure 4.3.4.3** Image analysis by persistent homology

**(2) Design of energy models by machine learning**

Machine learning such as Principal Component Analysis (PCA) and Ridge Regression are applied to magnetic domain structure data to analyze the relationship between structure and energy. This makes it possible to calculate energy barriers and analyze causal relationships in the magnetization reversal process.

Specifically, by integrating the features extracted by PH with machine learning models, it is possible to predict the time evolution of magnetic domain structures and magnetization reversal processes. In particular, by analyzing the correlation between changes in the persistence diagram and changes in the free energy, it is possible to clarify how magnetic wall migration and pinning phenomena are related to the energy barrier. By utilizing a highly interpretable machine learning model, the relationship between the formation and migration of magnetic walls and the energy topography can be analyzed in detail and the microscopic magnetic domain changes and macroscopic magnetic properties can be connected in a rational manner. This approach makes the relationship between magnetic domain structure and energy clearer and allows for optimization while physically interpreting the dynamics of iron loss and magnetization reversal.

**(3) Energy terrain analysis**

The obtained features are mapped on the information space to draw the energy topography (**Figure 4.3.4.4**). The analysis of energy topography is an important method for understanding the magnetization reversal process in detail. In particular, the extended Landau free energy model allows us to analyze the dynamics of magnetic wall migration and pinning phenomena by representing changes in the magnetic domain structure as an energy landscape.

Each point in the scatter diagram in **Figure 4.3.4.4** is a mapping of the magnetic domain structure in a certain state to the feature space, and the amount of movement of a point represents the amount of change in the magnetic domain structure in a time series. The larger the shift, the larger the update of the magnetic domain configuration. Since the total free energy is given to each point at the same time, the variation of the free energy required for the change of the magnetic domain structure can be visualized. For example, in the region on the right side of the figure, the total energy change is small despite the large movement of the data points. This region shows that the energy barrier is low and magnetization reversal occurs easily, indicating that it is a useful operating region for the operation of real materials in terms of low energy loss. Thus, the model can be used to quantitatively link the relationship of consumed (or stored) energy to changes in magnetic domain structure. This approach makes it possible to establish a relationship between the microscopic magnetic domain structure and the macroscopic magnetic function and to discuss the mechanism of iron loss quantitatively.

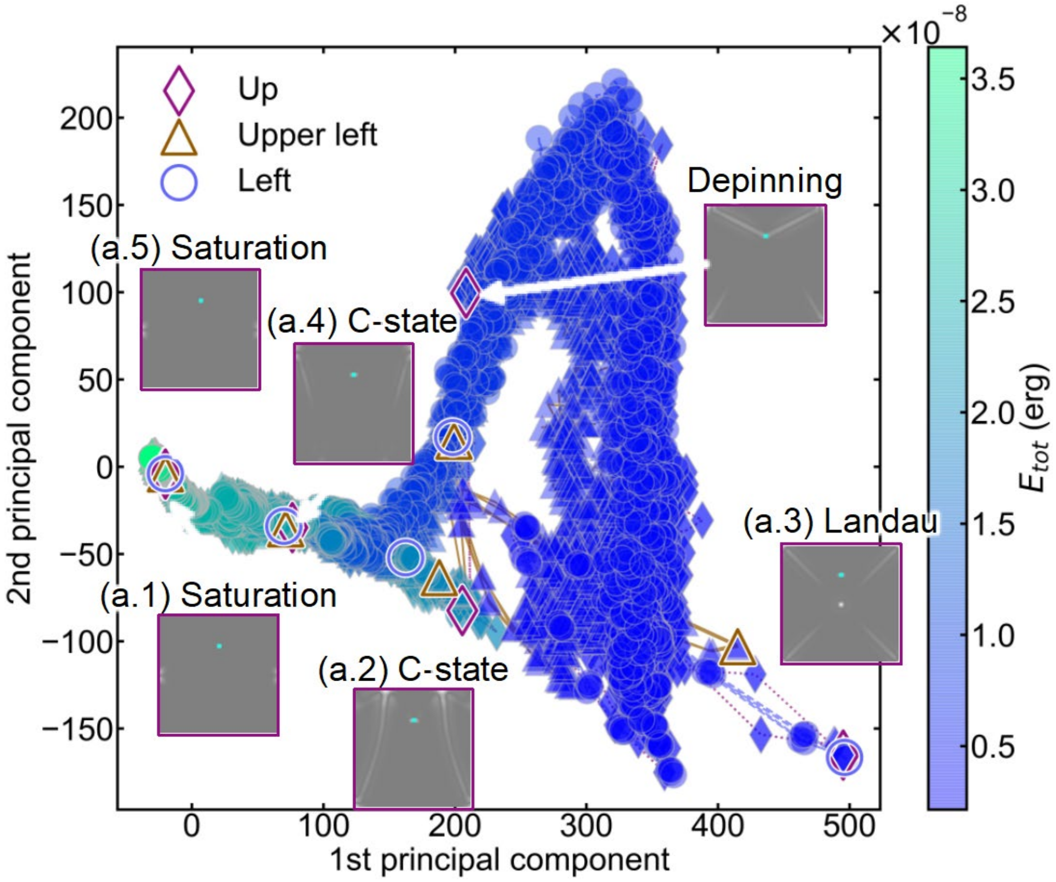


**Figure 4.3.4.4** Extended free energy model

Furthermore, by component decomposition of the magnetic free energy, it can be analyzed separately into magnetic wall and antimagnetic field components. Specifically, the mechanisms of magnetic wall movement and pinning phenomena can be analyzed. By focusing on the versatility of free energy, various energy terms can be incorporated, enabling multi-physics analysis. This physics-based model design enables us to obtain new knowledge in material design. By utilizing this method, we expect to clarify design guidelines for magnetic materials and contribute to the development of magnetic materials with optimal material properties.

**(4) Iron loss factor analysis by extracting energy barriers**

A differential analysis of the slope of the energy barrier provides a deeper analysis of the dominant factors in the pinning mechanism (**Figure 4.3.4.5**). This analysis method can also be applied to the factor analysis of iron loss. In particular, by quantitatively evaluating local changes in energy gradients, the energy loss associated with magnetic wall movement can be analyzed in detail and the physical factors contributing to iron loss can be clarified.

The energy barrier is an energy hurdle that must be overcome when a magnetic wall moves, and its size and distribution have a significant impact on the properties of magnetic materials. In the conventional Landau free energy model, the energy barrier, or effective field, is defined by differentiating the total energy by the magnetization of the order factor.

$$H_{eff} = -\frac{dE_{tot}}{dM} \tag{4.3.4.1}$$

On the other hand, in the present model, the total energy is differentiated by the characteristic of the structure (PC), which transforms the effective field as follows

$$H_{eff} = -\frac{\partial E_{tot}}{\partial PC} \cdot \frac{dPC}{dM} \tag{4.3.4.2}$$

The first term is the energy gradient in the information space, which directly provides an energy barrier to structural change. The second term is a proportionality coefficient that expresses the connection (correlation) between the features and magnetization, and can be absorbed as a constant by appropriate normalization, so detailed analysis and visualization can focus on the first term. Thus, the framework of evaluating barriers by differentiating the total energy by the characteristic quantities of the structure is a physics-based AI model that can handle the relationship between microstructure and macrofunction in an interpretable manner, while maintaining mathematical consistency (chain rule) with Landau theory.

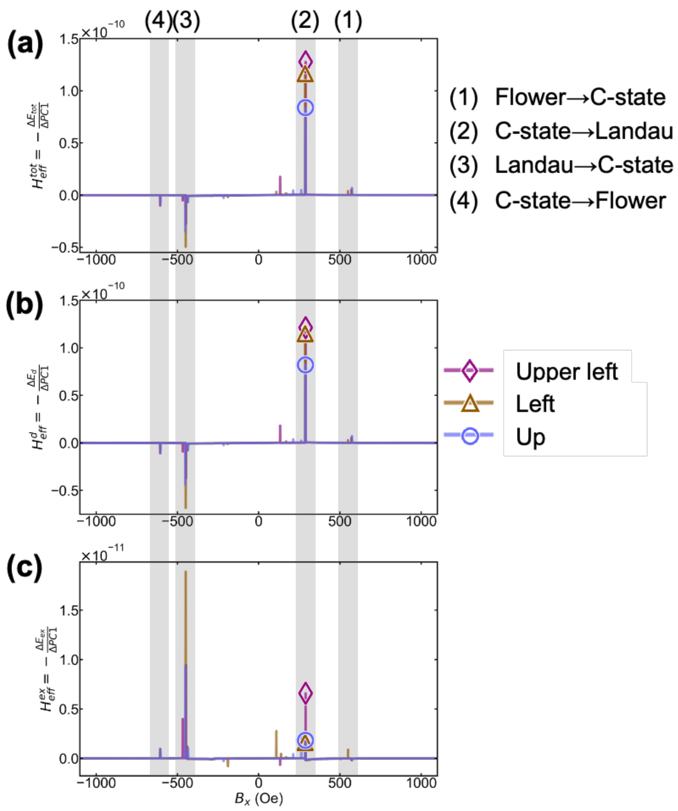


**Figure 4.3.4.5** Energy Gradient Analysis

**Figure 4.3.4.5** (a) shows the distribution of energy barriers derived from the total free energy. This allows us to quantitatively examine how the pinning of the magnetic wall is involved in the energy consumption (loss). In particular, a sharp peak around H ≈ 300 Oe is extracted as an outlier, which corresponds to the experimentally observed Barkhausen jump. Therefore, we show that this AI model can automatically identify and visualize the Barkhausen effect.

Furthermore, by performing component decomposition of anisotropy energy, exchange energy, and magnetostatic energy and clarifying their respective contributions, it is possible to identify which energy components inhibit or promote magnetic wall migration ( **Fig. 4.3.4.5** (b), (c)). As a result, it is clear that both magnetostatic energy and exchange energy contribute to the Barkhausen effect. At the energy barrier around -500 Oe, the magnetostatic energy and the exchange energy show opposite signs, indicating the antagonistic behavior of the two. This indicates that the promotion and inhibition of magnetization reversal cancel each other in the process leading to saturation.

Furthermore, attempts are being made to improve the prediction accuracy of iron loss by modeling changes in energy gradients using machine learning. In this method, features of the magnetic domain structure are extracted using PH, and by linking them to the free energy gradient, the mechanism of iron loss generation is analyzed in detail. While conventional methods evaluate the energy change based on time averages or simple empirical rules, this model differentiates the energy using the features of the structure, making it possible to clarify how the characteristics of local energy barriers and the pinning phenomenon of magnetic walls affect iron loss.

This approach allows us to directly link the causal relationship between local changes in magnetic domain structure and iron loss. Through the analysis of energy gradients, we can clarify which magnetic domain patterns increase iron loss and which conditions contribute to its reduction, thereby providing concrete guidelines for the optimal design of magnetic materials. In particular, the use of an explainable AI method makes it possible to statistically analyze microscopic structural factors affecting iron loss and visualize the results in a form that is intuitively understandable. This approach is expected to clarify design guidelines for magnetic materials to reduce iron loss and lead to the development of more efficient materials.

**(5) Visualization of iron loss factors**

Using the features obtained from the energy barrier analysis, the PD is reconstructed utilizing the Adamar product and projected onto the original magnetic domain structure ( **Figure 4.3.4.6** ). This method makes it possible to directly link the contributing factors of iron loss to the magnetic domain structure. First, in the energy barrier analysis, data on magnetic wall migration and Barkhausen jumps are collected, and their energy changes are extracted as characteristic quantities. These features are incorporated into the PD using a mathematical method called the Adamar product to visualize the relationship between the microscopic properties of the magnetic domain structure and the energy barrier. This approach allows detailed analysis of how magnetic wall migration and Barkhausen jumps contribute to the generation of iron loss. For example, it is possible to intuitively understand on the magnetic domain image whether a particular magnetic domain pattern is responsible for increasing the energy barrier or, conversely, has the effect of reducing iron loss.

**Figure 4.3.4.6** (a) shows the energy barriers described above reconstructed as PDs. This figure is the actual feature obtained by the Adamar product, which describes both the magnetic domain structure and energy information simultaneously; each generator of the PD can be back-analyzed to its original spatial coordinates, and the "loading factor" (contribution to loss) of all energies is visualized on the magnetic domain structure in **Figure 4.3.4.6** (b). The generators shown in blue are the regions that contribute to the energy loss, and the points can be compared quantitatively and visually. The analysis shows that the sample with the left defect (indicated by the point defect) has the lowest total number of generators and also the lowest number of generators in the vicinity of the defect. Furthermore, focusing on the magnetic wall, it was confirmed that the generators were distributed in three lines in the center of the magnetic wall and on the left and right sides of the wall. This indicates that the area contributing to the loss extends not only to the center of the magnetic wall but also to its periphery. Conventional visual analysis often considers the magnetic wall as a single boundary, but this result is a new finding obtained with the assistance of AI and encourages a reconsideration of the energy loss mechanism, including the role of the magnetic wall periphery.

This method enables detailed analysis of the relationship between defect location and magnetic domain shape for the pinning phenomenon in the Barkhausen effect. The Barkhausen effect is a phenomenon that occurs when magnetic domains move discontinuously, and is one of the important loss factors in iron loss. In this analysis, we were able to clarify the relationship between the location where the Barkhausen jump occurs and its energy barrier, automatically clarifying the location and origin of the Barkhausen effect. Specifically, it was shown that

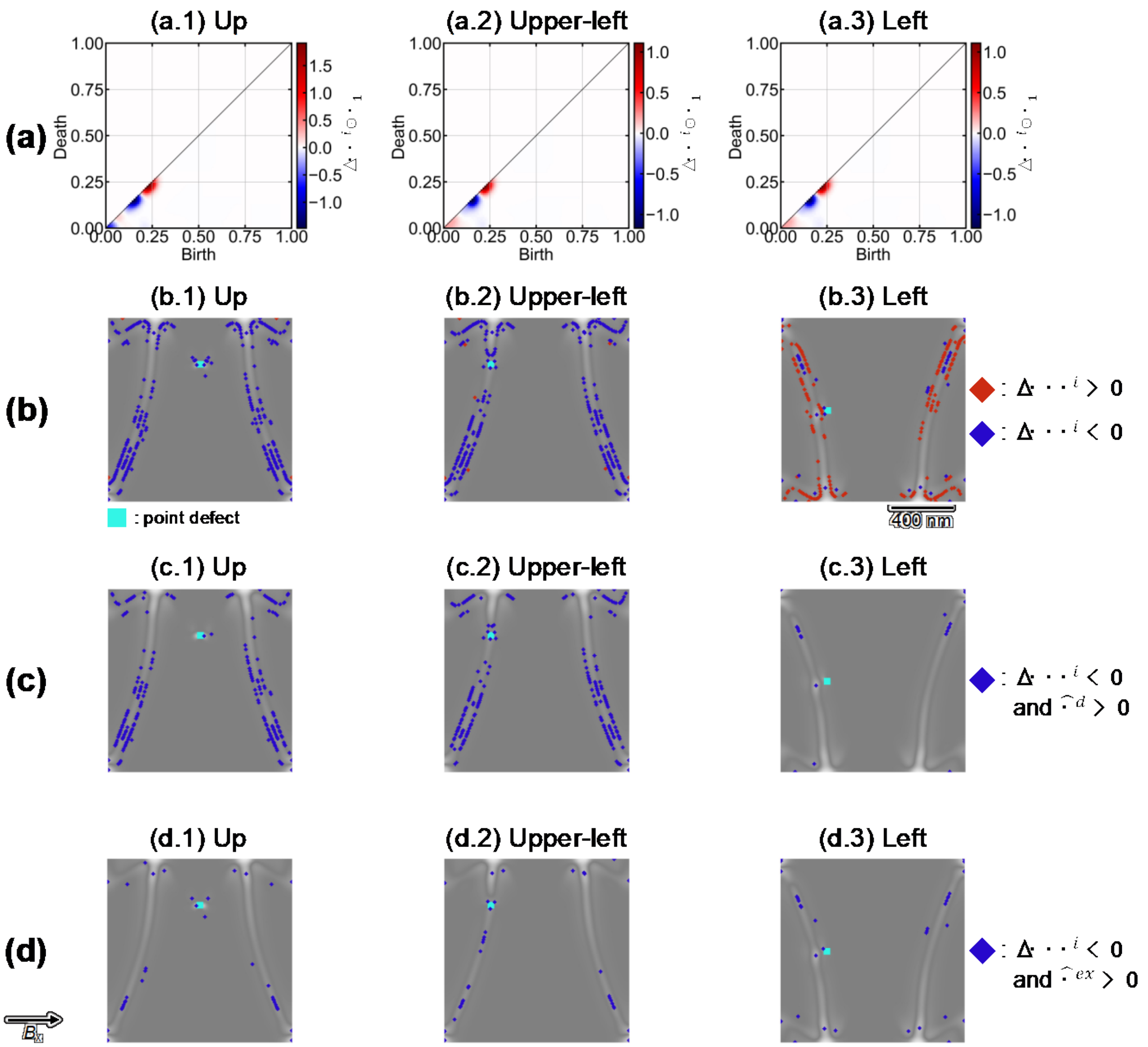


**Figure 4.3.4.6**

the rapid movement of the magnetic wall is induced depending on the defect location, which contributes to the increase in energy consumption.

In this analysis, the Adamar product is constructed for each energy term, and the results can be visualized. **Figures 4.3.4.6** (c) and (d) show an example of mapping each energy loading factor on the magnetic domain structure after decomposing the total energy into static and exchange energies. This allows the same visual and quantitative interpretation as described above.

For example, when comparing the number of generators, the sample with the defect position "Left" has the lowest magnetostatic energy, while the system with the defect position "Upper-left" has slightly less exchange energy The difference is observed in the exchange energy. Furthermore, quantitative evaluation of the energy loading shows that the contribution of the exchange energy is about two orders of magnitude smaller than that of the magnetostatic energy. In other words, the majority of the energy barriers are affected by the magnetostatic energy, which is directly involved in the movement of magnetic walls and pinning phenomena. In particular, it is clear that the static magnetic energy is a factor that forms localized pinning sites and causes discontinuous movement of magnetic domains. On the other hand, exchange energy was found to play an auxiliary role in magnetic wall migration and to act as a factor that promotes or suppresses magnetization reversal. In certain magnetic domain patterns, the exchange energy may locally increase and enhance pinning by suppressing magnetic wall migration. On the other hand, under certain conditions, the exchange energy distribution was observed to facilitate magnetization reversal by smoothing the movement of magnetic walls.

Focusing on defect placement, we can also see that the location of defects has a significant effect on the pinning characteristics. From the aforementioned energy comparison, we can also see that Left is the most desirable. In other words, the interaction between the magnetic wall and defects determines the pinning intensity and causes local variations in the energy barrier, as quantitatively evaluated through the analysis. In particular, it was confirmed that the energy barrier becomes higher in the region where defects exist, and the movement of the magnetic wall is suppressed. This suggests that the local energy barrier due to defects contributes significantly to the stability of the magnetic domain structure. This method provides a logical interpretation of the loss mechanism and a guideline for the optimal material structure.

Visualization of energy barriers is an important guideline in material design. In the optimization of magnetic materials for the purpose of reducing iron loss, clarifying what kind of magnetic domain structure is desirable will enable more efficient material design. Furthermore, it is expected that the relationship between changes in magnetic domain structure and iron loss can be automatically learned and used in combination with machine learning to support the design of optimal magnetic materials. Future research should apply these methods to the optimal design of a wider range of magnetic materials and to the development of passive components for the purpose of reducing iron loss.

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## 3.5 Applied research on extended free energy models: examples

**Keyword:** Non-oriented electromagnetic steel sheet, Thermal stability analysis, Entropy

### 3.5.1 Magnetic Domain Structure Analysis of Non-Oriented Magnetic Steel Sheets

Energy loss in nonoriented electromagnetic steel sheets (NOES) is an important issue that directly affects the efficiency improvement of electric motors [1]. In this section, an extended free energy model is applied to the magnetic domain structure of NOES to reveal the microscopic origin of energy loss ( **Figure 4.3.5.1**) [2].

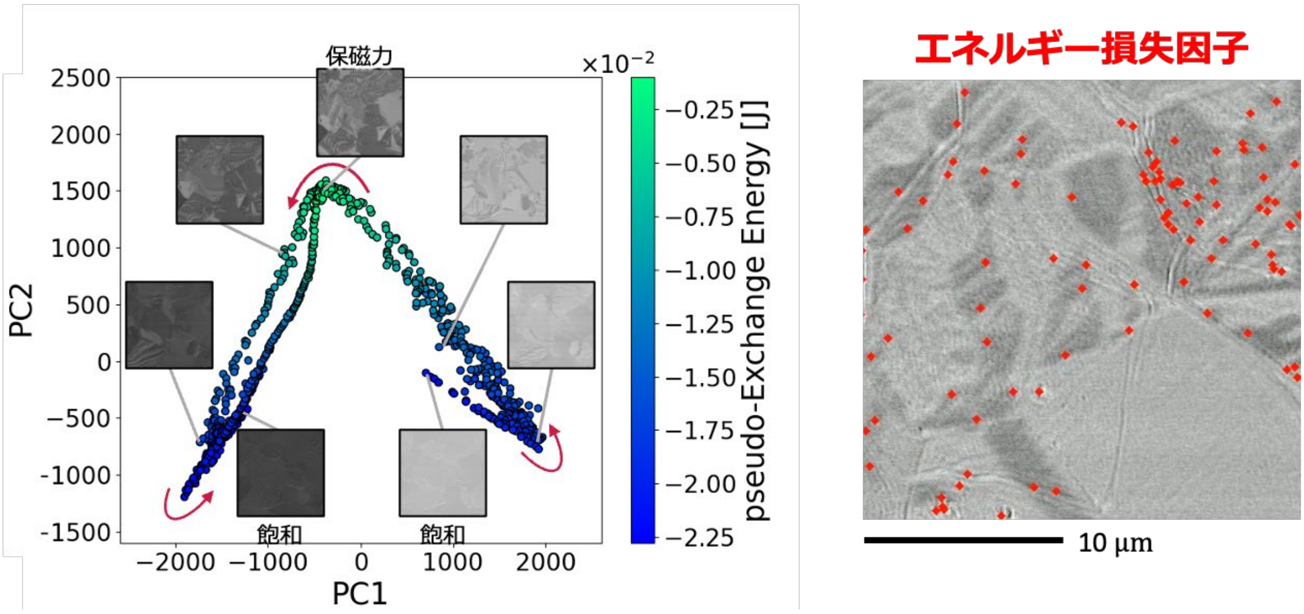


**Figure 4.3.5.1** Analysis results of extended free energy in omnidirectional electromagnetic steel sheet

In this study, experimental magnetic domain images acquired by Kerr microscopy were used as input data. The configuration of the extended free energy model is the same as in the previous section, and its application to the experimental data was smooth because the robustness of the model was verified in advance with computational data. The obtained energy topography shows that the data points of each magnetic field move along a smooth trajectory in PCA space as the magnetization reversal progresses, and that the magnetic domain structure and magnetic wall energy changes are continuous. These results indicate that the typical magnetization reversal process of soft magnetic materials is adequately captured. PC1 shows a monotonous linear relationship with magnetization and functions as an explanatory variable for macroscopic magnetization. On the other hand, PC2 shows a high correlation with the magnetic wall energy (exchange energy) and is found to be a variable that explains the energy and shape of the magnetic wall well. This provides a basis for connecting the relationship between the microscopic magnetic domain structure and the macroscopic magnetic wall energy.

The factors contributing to the magnetic wall energy were then visualized on the magnetic domain structure: the eigenvectors of PC2 and the Adamar product of the persistence diagram were constructed, the energy loss factors were defined, and mapped onto the original magnetic domain structure. This allows us to specify which regions inhibit the movement of magnetic walls. The visualization results clearly show that the grain boundaries contribute strongly to the pinning, with high-density generators densely accumulated in the vicinity of the grain boundaries. Furthermore, focusing on the inside of the grains, a series of generators along a particular magnetic wall indicates the existence of a magnetic wall that suppresses inversion. On the other hand, magnetic walls with almost no generators were also observed. In other words, there are magnetic walls that contribute to energy loss and magnetic walls that contribute little to energy loss, and it is possible to classify them according to their different roles. A movie of the visualization results can be found in Reference (2). This classification is a new knowledge obtained by physics-based AI, and it further deepens our understanding of the magnetization reversal mechanism.

In general, the extended free energy model links "structure-mechanism-function" in an interpretable manner and clearly depicts the contribution of magnetic walls associated with pinning near grain boundaries and segmented magnetic domains within grains. This allows us to identify both the location (where it occurs) and the mechanism (which type of magnetic wall is responsible) that contribute to hysteresis loss in NOES, and provides practical guidelines for material design and process optimization. The results of this research can be applied not only to the reduction of iron loss in NOES, but also to the analysis and optimization of other non-homogeneous magnetic materials. Further introduction of machine learning techniques is expected to improve the accuracy of interpretation of the energy landscape, and it is expected to be used as a design guideline for magnetic materials.

#### 3.5.2 Visualization of coercivity factors in soft magnetic materials: analysis by magnetic wall motion and topological data analysis

Detailed analysis of magnetic wall motion is underway to elucidate the factors that generate the coercive force during the magnetization reversal process of soft magnetic materials [3]. As a method to observe the dynamics of magnetic domain structures in real time, a measurement technique combining a magneto-optical Kerr microscope (MOKE) and a high-speed camera has been utilized, and the response of magnetic domains to changes in external magnetic field has been recorded with high precision. Furthermore, by using persistent homology (PH), a method of topological data analysis (TDA), changes in magnetic domain structure were quantified numerically, and combined with principal component analysis (PCA), the characteristics of the magnetization reversal process were extracted. The results clearly show the influence of magnetic wall motion on coercivity and indicate that a specific magnetic domain structure is a factor that suppresses magnetization reversal. In particular, the change in coercive force under high-frequency magnetic fields was visualized, and the effect of the microscopic structure of magnetic domains on energy loss was quantitatively evaluated. This finding provides a design guideline for controlling coercivity and reducing energy loss in soft magnetic materials and may contribute to the development of higher performance magnetic materials. For details, please refer to the open-access description in Ref.

#### 3.5.3 Analysis of thermal stability of magnetization state and magnetization reversal field by Landau theory

Methods to reduce the magnetization reversal field while maintaining the thermal stability of the magnetization state have been analyzed based on Landau theory [(4)]. Although increasing or decreasing the magnetic anisotropy energy has been an issue that creates a tradeoff between thermal stability and recording performance, flattening the energy landscape by joining the soft and hard phases has attracted attention as an effective method. In particular, an analysis of the effect of the inclined shape of the energy landscape on the magnetization reversal field has shown that an energy landscape with linearly inclined energy topography is optimal. The reduction of the energy barrier with increasing temperature and the effect of entropy on the magnetization reversal process were quantitatively evaluated, and it was found that magnetization reversal at low magnetic fields can be achieved without compromising magnetization stability by designing appropriate energy landscapes. This method is useful not only for improving the performance of magnetic recording media, but also as a design guideline for new magnetic materials. Furthermore, it is expected that optimization of the energy topography considering the temperature dependence will enable the maintenance of a more stable magnetization state. For details, please refer to the open-access article (4).

#### 3.5.4 Super-hierarchical and explainable analysis of magnetization reversal processes using topological data analysis

Detailed analysis of the changes in magnetic domain structure and the magnetization reversal process is essential to improve the performance of spintronics devices. In this study, we developed a super-hierarchical and explainable analysis method of the magnetization reversal process by utilizing topological data analysis (TDA)[(5)]. The complexity of the magnetic domain structure was quantified using persistent homology (PH), and the characteristic quantities of the magnetization reversal process were extracted through visualization in a low-dimensional space by principal component analysis (PCA). As a result, it was found that the first principal component (PC1) represents the magnetization change, and the second principal component (PC2) characterizes the stability of the magnetic domain structure. Furthermore, by analyzing PC2, we identified branching factors in the magnetization reversal process in stable and metastable states, and deepened our understanding of the stochastic and deterministic properties of magnetization reversal. This method clarifies the hierarchical relationship between magnetic domain structure and magnetic function, and is expected to be applied to improve the reliability of spintronics devices and to guide the design of new devices. For details, please refer to the open-access article (5).

#### 3.5.5 Study of structural features and connection of computed and experimental data

It is important to consider structural features in extended free energy models. In this study, Fourier transform (FFT) was utilized to analyze the characteristics of the magnetization reversal process while preserving the periodicity of the magnetic domain structure [(6)]. Principal component analysis (PCA) was utilized to embed the features of the magnetic domain structure in a low-dimensional space and correlate them with hysteresis loops. The analysis showed that there is a pattern in the feature space in which magnetization and exchange energy are strongly correlated, which reflects the coercive force. Similar trends were observed in both simulations and experiments, confirming the reliability of the energy landscape. This method enables visualization using physical features, which can be used to identify energy barriers in the magnetization reversal process and to understand the origin of the coercivity in more detail. Furthermore, the data transformation using FFT preserves information on the periodic magnetic domain structure, thus extending the Landau theory. This will allow us to better understand the coercive force mechanism while taking into account inhomogeneities in actual materials, and is expected to be applied to the design of the next generation of soft magnetic materials. For details, please refer to the open-access article (6).

These studies represent the forefront of magnetic materials analysis utilizing extended free energy models and materials informatics, and are expected to contribute to further research in the future.

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## 3.6 Summary and Future Issues

In this paper, we introduce the extended Landau free energy model as a new method for magnetic materials analysis utilizing materials informatics. It is shown that it is possible to analyze in detail the properties of magnetic domain structures and energy barriers that cannot be captured by conventional analysis methods using a data-driven approach, and to evaluate the microscopic magnetic domain structures and macroscopic magnetic functions in an integrated manner.

In the analysis of the magnetization reversal process, feature extraction of magnetic domain structure, visualization of energy barriers, and automatic analysis of pinning phenomena were realized by using persistent homology. By component decomposition of energy, we were able to separate the contributions of magnetostatic energy and exchange energy and clarify the role of each. This enabled a deeper understanding of the mechanism of the pinning phenomenon and quantitative identification of the factors that cause iron loss.

The knowledge obtained in this study provides guidelines for the optimal design of magnetic materials and contributes to the development of highly efficient magnetic materials for the purpose of iron loss reduction. In particular, through the analysis of energy topography, the effects of defect location and magnetic wall migration characteristics on the energy barrier were quantitatively evaluated, providing concrete knowledge for the design of optimal magnetic domain structures.

These results are particularly important in the materials design of passive components for power electronics. Power electronics is a core technology for power conversion and control, and the properties of magnetic materials used in power electronics greatly affect the efficiency and reliability of the devices. The analytical methods used in this study will not only promote the development of soft magnetic materials with low iron loss and high permeability, but also contribute to the reduction of power loss and improvement of operational stability in passive components.

Specifically, optimization of the magnetic domain structure is expected to reduce core losses in transformers and inductors, resulting in more efficient power conversion. In addition, detailed analysis of the energy topography is expected to provide design guidelines for controlling the behavior of magnetic wall movement and suppressing losses in high-frequency environments. In particular, through the analysis of magneto-elastic energy, the influence of magnetostriction on the magnetic domain structure can be quantitatively evaluated and design guidelines that take into account the stress dependence of magnetic materials can be provided. Furthermore, by analyzing the energy topography from the viewpoint of dynamics in terms of high-frequency response, it is expected to clarify the time dependence of magnetic wall migration and the characteristics of energy consumption under high-frequency magnetic fields. These analyses will provide a new guideline for material design to reduce losses during high-frequency operation in power electronics.

These developments will accelerate the development of high functionality in magnetic materials and contribute to the improvement of energy efficiency in the next generation. The method established in this study can be applied not only to magnetic materials but also to the design of other functional materials, and is expected to develop as an innovative analysis method in a wide range of materials science fields.
[Masato Kotsugi, Takahiro Yamazaki]

# Section 4 Utilization of Machine Learning for the Development of Magnetic Materials and Magnetic Elements

## 4.1 Machine Learning for Development of Passive components Using Soft Magnetic Materials

**Keyword:** Machine learning, Soft magnetic material, Property prediction, Database, Inverse problem analysis, Integrated design

Power electronic circuits (power electronics circuits) are becoming higher frequency, smaller, and more efficient by utilizing power semiconductors made of new materials such as silicon carbide (SiC) and gallium nitride (GaN) [(1)-(3)]. On the other hand, the development of low-loss magnetic elements such as transformers and inductors in the high-frequency band is a challenge, and the creation of low-loss magnetic core materials in addition to the required magnetic permeability and saturation density in the high-frequency band is required [(4)].

Material development has been conducted to reduce loss while maintaining the required properties such as magnetic permeability and saturation flux density in the target frequency band [(5)-( 10)]. The development of low-loss materials has always been a major challenge, and various mathematical models have been proposed to analyze the mechanism of loss generation. Among them, Steinmetz's experimental equation [(11)], proposed in 1892, is still used as an index for material development. This equation separates the losses occurring in the magnetic core through fitting with experimental values into three categories: hysteresis loss, anomaly loss, and eddy current loss. This makes it possible to consider guidelines for material design. However, its application is limited and must be supplemented by knowledge and experience in order to use it correctly. There are attempts [(12)( 13)] to add parameters such as operating temperature, frequency, excitation waveform, and amplitude in order to expand the range of application, but the large-scale measurement and analysis is an issue.

Against this background, new approaches have recently been proposed to estimate and analyze AC losses using machine learning [(14)-( 16)], and open source databases that collect waveform data measured under multiple operating conditions for various magnetic cores have been published.

The application of machine learning in the development of magnetic materials and magnetic elements is currently at the stage of introducing data-driven development. In the future, it is important to establish a foundation for the development of autonomous magnetic materials and magnetic elements that do not require prototyping and for the development of integrated design technology with circuits. Specifically, data on process parameters, material properties, electromagnetic properties, and performance should be collected and organized, and techniques to eliminate individual differences and measurement errors in the data should be established. Then, a system will be established to predict material properties such as structure, saturation flux density, loss, and magnetic permeability, and to provide feedback to each process. In the next stage, this inverse problem analysis will enable optimization methods for process parameters and other parameters to be made more accurate and integrated design with circuits to be realized, thus accelerating prototype-less development. If this optimization method and the actual process are seamlessly linked, the discovery of high-performance materials through autonomous design will be realized. In addition to parameters related to the performance of power electronics circuits, parameters related to electromagnetic compatibility, sustainability, and environmental resistance could also be considered for multi-objective design.

In this section, we present a concrete example of the introduction stage of data-driven development as a case study of the use of machine learning for the development of soft magnetic materials and magnetic elements. One of the main objectives of the introduction phase of data-driven development is to establish a new approach to materials design that does not rely on conventional empirical rules by making full use of supervised and unsupervised learning, paving the way for process optimization and autonomous design.

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## 4.2 Case study of analysis of magnetic materials using machine learning

**Keywords:** nanocrystalline soft magnetic materials, gradient boosting, factor analysis, loss prediction, inverse problem analysis, Bayesian inference, generative model, magnetic wall migration

### 4.2.1 Analysis Examples

We present a case study of the use of machine learning to reduce the loss of soft magnetic materials in which fine α-Fe particles are precipitated from amorphous materials. From 1294 data in related previous papers and 160 data from our own experiments, we collected as features: material composition, process conditions such as heat treatment temperature and time, α-Fe grain size determined from transmission electron microscopy, microstructure information such as volume fraction obtained from atom probe analysis as shown in Section 1.3.5 of Chapter 2, coercive force the machine learning was conducted using the gradient boosting method with coercive force and loss as the objective variables. As an example of the results, **Figure 4.4.2.1** shows a comparison of the experimental values of loss and the prediction results by machine learning. The results show that the predicted values and experimental values are relatively well aligned, indicating that good predictions were made. In addition, we analyzed the factors of additive elements and heat treatment conditions on the important characteristics such as coercive force, saturation magnetization, and loss ( **Figure 4.4.2.2**, example of correlation coefficient), and optimized the additive elements and heat treatment conditions using these analysis results as guidelines.

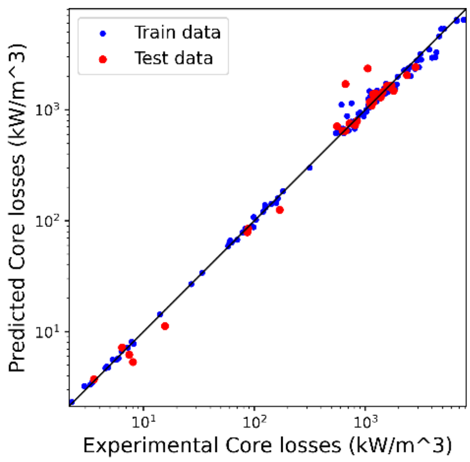



**Figure 4.4.2.1** Example of comparison between experimental loss and machine learning prediction results

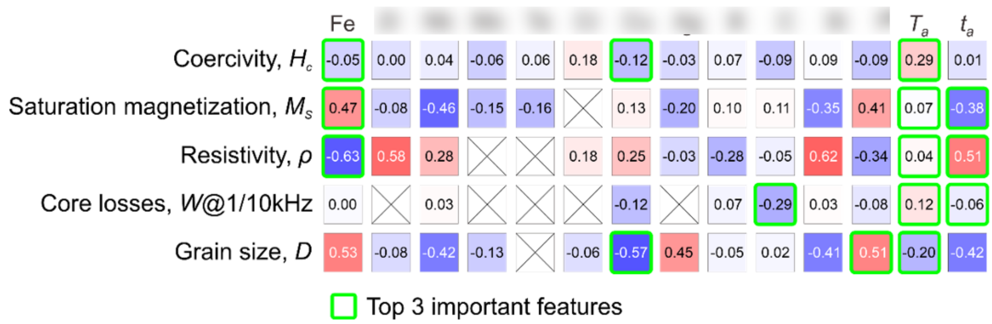



**Figure 4.4.2.2** Results of factor analysis of representative features

### 4.2.2 Possibilities for material property improvement and inverse problem analysis

Regarding the possibility of improving material properties, new guidelines are being found for reducing iron loss. Until recently, it has been assumed that nanocrystalline soft magnetic materials are crystallized with a high volume fraction of α-Fe. Recently, however, it has become clear that excellent low iron loss can be obtained in the region where the volume fraction of α-Fe is a few percent (PCT/JP2023/042606). Recent magnetic domain image observations suggest that magnetic wall migration is suppressed in low iron loss samples, and that magnetization reversal occurs mainly by rotation of the magnetization vector. In other words, suppression of magnetic wall movement and promotion of rotational magnetization are thought to contribute directly to iron loss reduction. In order to actively achieve this, the imposition of magnetic anisotropy and the formation of a microstructure with structural and magnetic fluctuations are considered to be effective, and future research is awaited.

Regarding the possibility of inverse problem analysis, material/process conditions, microstructure, and magnetic domain structure are important factors in determining properties, and adjusting these factors significantly changes the properties obtained. In order to understand the correlation between these many parameters and properties, it is important to accumulate experimental data along the flow of material/process conditions → microstructure → magnetic domain structure → properties, and then, after integrating simulation data, construct and advance an inverse problem analysis system that utilizes machine learning to clarify the direct correlation between each factor. The first step is to clarify the direct correlation between each factor. As the next step, it is necessary to set a target property, for example, the value of iron loss, and conduct an inverse problem analysis to achieve it. In this analysis, the objective is to clarify the magnetic domain structure and microstructure to obtain the required properties, and finally to propose appropriate material and process conditions. Since the inverse prediction usually involves multiple possibilities, it is important to efficiently search for the optimal solution within the constraints. In this case, it is necessary to use Bayesian inference and generative models to efficiently narrow down promising candidates from a wide range of search regions. These methods will enable further development of low iron loss materials through inverse problem analysis.

## 4.3 Case study of analysis of magnetic elements using machine learning

**Keyword:** Powder core, Surrogate model, Gaussian process (GP), Target value driven design, EMC design, Integrated design

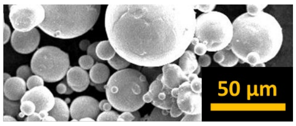
#### 4.3.1 Analysis Examples

Aiming to construct an optimization system for process conditions with a target performance value for iron-based pressed magnetic cores, this paper presents a case study of prototyping and measuring pressed magnetic cores using electrolytic iron powders with different process conditions and using machine learning of the data to estimate the AC losses of the magnetic cores. The objective of this approach is to replace the physical process, which is very costly in terms of experimentation and evaluation, with a surrogate model. The surrogate model is a mathematical model that predicts an objective variable (output or result) from explanatory variables (inputs or conditions). To construct the model, a regression model was trained by organizing the data set of trial conditions, measurement conditions, and measured AC loss values of the magnetic core. The regression model was the Gaussian Process (GP) model [(1)], which is widely used for learning small amounts of data.

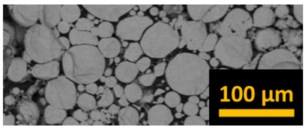
The sample used for the evaluation was a magnetic powder core consisting of spherical electrolytic iron particles [(2)]. **Figure 4.4.3.** 1 shows SEM images of the electrolytic iron powder used and the cross section of the magnetic core produced. The particle diameter $D_{50}$ ranges from 10 to 40 μm, and it can be seen that a densely packed structure is formed with the individual particles maintaining their original shape. Particles of each diameter were insulated with 0.3 to 3.0 wt.% silicone and formed into a ring shape using a mold at a pressure of 10 ton/cm$^2$. The ring was then heat-treated at 500 to 900 ℃ for 2 hours. The finished cores have an outer diameter of 13 mm, an inner diameter of 8 mm, and a height of approximately 5 mm.

Process conditions (particle size, resin blend ratio, and annealing temperature) and loss measurement conditions (frequency 1 kHz to 4 MHz, amplitude of applied flux density 1 to 100 mT) for 40 different magnetic cores with different process conditions were used as explanatory variables. The objective variable was the measured AC loss [(2)]. The data set consisted of a total of 1900 data sets. Here, based on the knowledge of Steinmetz's experimental formula that AC losses can be approximated by a power law of frequency and applied flux density, a part of the data set was converted to logarithms. Only the data set for a particular magnetic core (about 5% of the total) was used for testing, and the regressor was trained using all the rest.

**Figure 4.4.3.2** shows an example of predicted and experimental AC losses by GP regression as a function of frequency and applied flux density in a three-dimensional graph. The figure shows that the predicted values are in very good agreement with the experimental values under a wide range of measurement conditions, from low to high frequencies and from low to high flux densities, demonstrating that a highly accurate surrogate model incorporating the knowledge of physical laws can be constructed.




(a) SEM image of




(b) SEM image of magnetic core cross section

**Figure 4.4.3.1** SEM image of electrolytic iron powder and cross section of magnetic core with

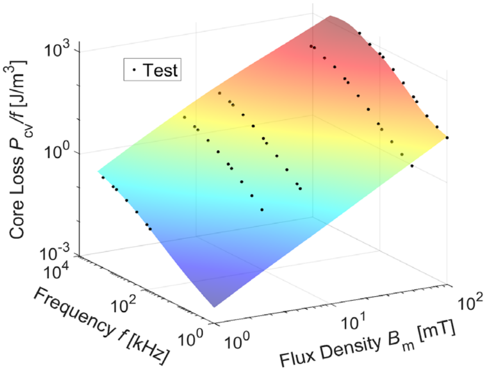



**Figure 4.4.3.2** Example of AC loss estimation

### 4.3.2 Possibility of constructing material design guidelines with device performance as a target value

The highly accurate surrogate model demonstrated in Section 4.3.1 (previous section) is the first step toward accelerating materials development. However, in order to transform the model into a truly practical goal-driven design system, it is necessary to address two major issues: expansion of the model's "scope of application" and "integration" with design systems in other fields.

Although this surrogate model has high prediction accuracy for the specific magnetic powder core material system used for training, it cannot predict the performance of materials with different compositions or unknown new materials. To overcome this limitation and enable a more universal material search, the surrogate model can be linked to a material database, and the composition of the material itself (type and ratio of elements) can be incorporated into the model as an explanatory variable (input data). It is expected that by linking with a huge material database, it will be possible to propose new material compositions to satisfy target properties.

In addition, optimization of materials alone does not necessarily maximize the performance of the device as a whole. Therefore, the realization of cooperative and integrated design between material development and circuit design is an important step. In particular, for high-speed switching circuits using next-generation semiconductors such as SiC and GaN, not only optimization of efficiency and size, but also EMC design is an important factor, requiring the development of high-performance magnetic materials that appropriately suppress, reduce, or shield electromagnetic noise outflow.

To realize this, it is expected that an integrated system will be constructed to propose optimal "materials," "circuit and device structures," and "selection and arrangement of noise suppression components" by linking the constructed surrogate model with circuit optimization systems and electromagnetic field simulations.

[Sho Muroga]

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