Market Research on Electrical Motor and Power Electronics Technology and Magnetic Material Multi-Scale Analysis

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電気モータで駆動する自動車や飛行機の EV 社会，パワーエレクトロニクス技術を介してエネルギーが利用されるパワエレ社会が進展している． 図 1 は，2030 年の EV やその関連装置およびパワーエレクトロニクス装置の世界的市場規模を調査した結果を示したものである [1]. エアコンおよび EV に大きな市場が見込めるが，特にワイヤレス充電システムの市場規模が著しい．

そこには多くの磁性材料が使用されており，これまでにない新たな動作領域での磁性材料が必要とされる．特に GaN，SiC デバイスによる高周波大電力動作に対する新たな磁性体へのニーズは高い．そこでは，MHz, 100 kW を超えるものも予想され，変位電流と磁気飽和による非線形現象との同時発生が起こりえる．そうした材料開発およびパワーエレクトロニクス回路での利用技術では，磁気の根源・物理現象に根差した解析技術つまり図２のごとき磁性体マルチスケール解析技術を踏まえての開発，研究が必要と思われる [2, 3].

これまでのエネルギー系の商用周波数での磁気論は，100 年以上の時間をかけて磁気関係者が量子論や磁区構造論，多結晶論などを陽に表すことなく電気関係者に提示してきた．しかし高周波大電力動作が急速に実用化しようとしている現在，ある意味不完全な材料，開発途上の材料が，電気関係者が利用しなければいけない状況になっている．パワエレ磁気では使用する部位によって動作している磁気特性が異なるため，磁気関係者にはその状況であることを踏まえていただくと同時に，早急な材料開発及び利用技術の深展のための支援技術となる各磁気現象における解析技術について熟知すべきと思いで，本シンポジウムを開催する．

(a)　EV, PHV 向け充電インフラの市場規模　　(b)　パワエレ装置の市場規模

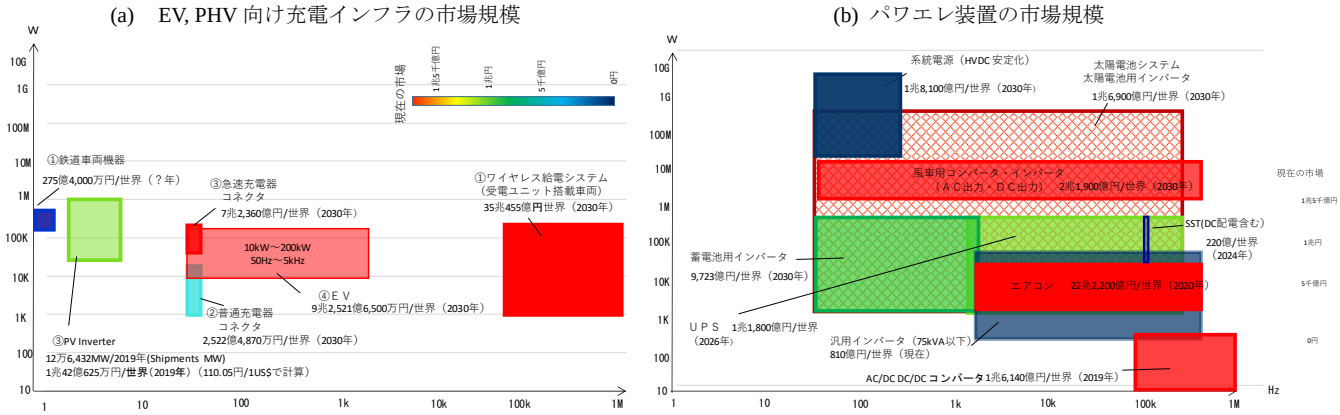

図１．世界市場調査結果（2030 年の予測）[1]

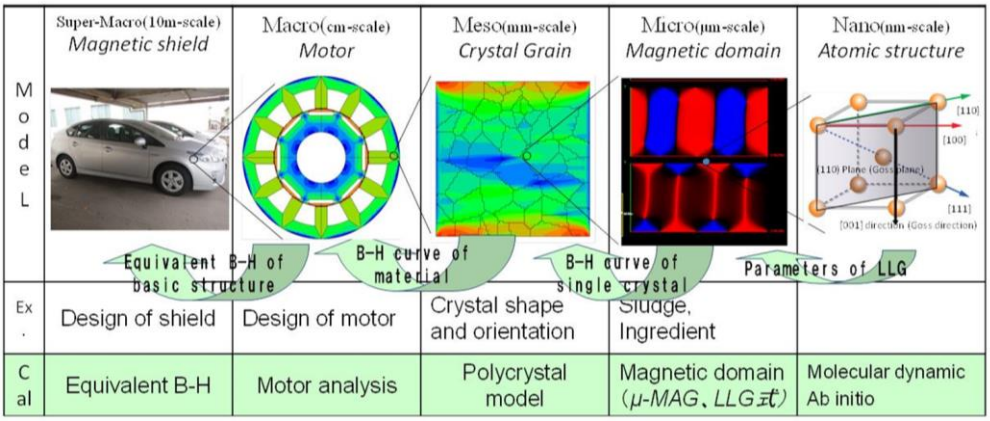

図２．磁性体マルチスケール解析技術 [2, 3]

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講 演 取 消

Investigation of iron-rich FeSi alloys by first-principles phase field and special quasirandom structure methods

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Fe-6.5 wt% Si has special magnetic characteristics as zero magnetostriction, low magnetic anisotropy, low iron-loss, and high magnetic permeability.[1,2)] It is possible to infer that the low iron-loss is due to the increase of electric resistance with silicon, and that the high magnetic permeability is due to the reduction of magnetic anisotropy. However, it has not been discussed enough in the literature why zero magnetostriction and low magnetic anisotropy appear at the special composition of the FeSi alloy. When magnetic materials are processed into devices such as motors, transformers, and inductors, mechanical stress applied results in residual stress, which deteriorates the magnetic properties. Therefore, the magnetic material which shows zero magnetostriction is very attractive. If a material with zero magnetostriction can be developed, devices with low iron-loss and high magnetic permeability can be realized, leading to miniaturization and high efficiency, which can contribute to realizing power electronics society.

In this study[3)], coarse grained phase morphologies of iron-rich region of FeSi alloys at 1050 K are investigated by using first-principles phase field (FPPF) (Fig. 1) and special quasirandom structure (SQS) (Fig. 2) methods without relying on any experimental or empirical information. From the free energy comparison, we find that, for the Si concentration less than 25 at%, a solid-solution-like homogeneous phase is most stable, although a random pattern in nm scale consisting of B2 $Fe_{4-x}Si_x$ and $D0_3$ Fe_3Si phases may appear at 12.5 at% Si at somewhat lower temperatures. We make a conjecture that, around 12.5 at% Si, such a random pattern in nm scale is the origin of the zero magnetostriction and low magnetic anisotropy. This solves a long-standing problem of the experimentally observed zero magnetostriction at 6.5 wt% Si. On the other hand, for the Si concentration slightly larger than 25 at%, FeSi alloys prefer two-phase coexistence of the $D0_3$ Fe_3Si phase and the B2 FeSi phase. All these findings are in good accordance with the available experimental evidence.

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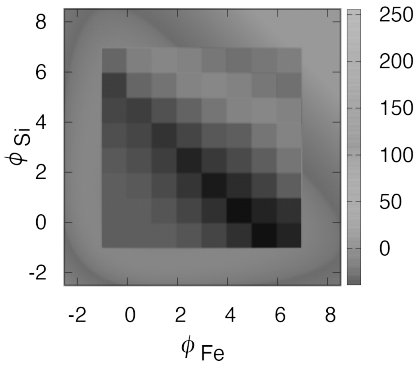

Fig. 1 2D Free Energy Map of the FPPF Method

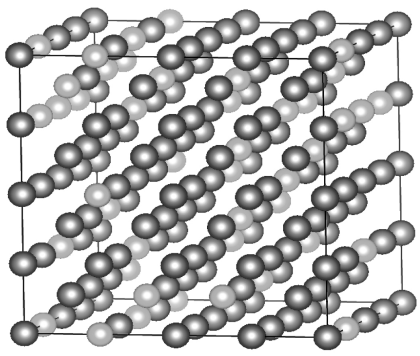

Fig. 2 Random Atomic Configuration in the SQS Method

A trial to evaluate the magnetic parameters in the LLG equation from the first principles

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Ultimate purpose of the first principles calculations is to predict physical and/or chemical properties, in a quantitative level, of materials and then to design newly developed materials. To achieve this mission, the first stage we should attain is to reproduce the measured properties of solids and molecules. However, as is widely recognized in materials science, even this level is currently hard to be reached. One reason lies in a fact that the material characteristics are governed not only by their microscopic (physical) features but also by macroscopic properties which in many cases dominate the performance of industrial materials. In the current stage, the first principles approach can contribute only to the former (microscopic) properties which can be treated based on the quantum physics. Especially, in the fields of magnetism and superconductivity, the first principles studies are limited to the subjects related to the formation of the order parameters, magnetization and macroscopic wavefunction, respectively. Once an order parameters is built up through the phase transition, the macroscopic properties can be handled using the order parameter as a phenomenological parameter as in the Ginzburg-Landau theory for superconductivity and the Landau-Lifshitz-Gilbert (LLG) equation for micromagnetics. In a ferromagnetic system, for example, spin operators can be treated as classical vectors, $\boldsymbol{M}$ in the magnetic Hamiltonian, $H(\boldsymbol{M})$, and the LLG equation is given by

$$\dot{\boldsymbol{M}} = -\gamma \boldsymbol{M} \times \boldsymbol{H}_{eff} + \left(\frac{\alpha}{M}\right)\dot{\boldsymbol{M}} \times \boldsymbol{M}, \qquad \boldsymbol{H}_{eff} = -\frac{\partial H(\boldsymbol{M})}{\partial \boldsymbol{M}}$$

In this stage, the first principles calculation can contribute to provide the magnetic parameters, such as magnetization $\boldsymbol{M}$, exchange constant J_{ij}, anisotropy constant K_i, and the Gilbert damping constant α. One should note here that first principles study can, in principle, determine these parameters only at $T = 0$, whereas the desired properties are mainly at finite temperatures.

To overcome this situation, we have recently made a trial to calculate the temperature dependence of the magnetic parameters, $M(T)$, $A(T)$, $K(T)$ and $\alpha(T)$, within the frame of the first principles technique.[1-4] A method for $M(T)$ and the anisotropy constant $K(T)$ at finite temperature have been developed by Staunton *et al.*[5] based on the functional integral method combined with the disordered-local-moment approach. We extend this method to analyze exchange stiffness constant $A(T)$ and $\alpha(T)$, and further developed a perturbation theory and linear response theory at $T \neq 0$. Here, we evaluate $A(T)$ by estimating the excitation energy of the spirally twisted spin structures.

In this symposium, we will present the theoretical framework and show some calculated results of the magnetic parameters of transition metals and alloys

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Magnetic moment and magnetocrystalline anisotropy energy of Fe, Ni, and Co using first-principles calculations

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In recent years, with the development of computer technology, research and development of magnetic materials and devices has increasingly relied on various computer simulation methods. Representative methods include first-principles calculations at the atomic level, micromagnetic calculations using the Landau–Lifshitz–Gilbert (LLG) equation at the micro level, and electromagnetic field calculations using Maxwell equations that can handle sizes larger than the millimeter level. First-principles calculations analyze electronic states and energies. For example, in the field of magnetism, saturation magnetization (magnetic moment), magnetocrystalline anisotropy energy (MAE), and exchange stiffness can be obtained without using experimental values. Additionally, M-H loops and magnetization behavior can be obtained using the LLG equation. Electromagnetic field analysis using Maxwell equations can analyze the magnetic flux flow due to the interaction of electromagnetic fields. Thus, multiscale analysis, where atomic-level analysis information (magnetic characteristics) is input to LLG equation, and the analysis information (M-H loops) of LLG equation is input to Maxwell equations, will become increasingly important in the future.

Therefore, in this study, to obtain the input parameters of the LLG equation from first-principles calculations, the magnetic moments of Fe, Ni, and Co [μ_B/atom] ($\mu_B = 1.165 \times 10^{-29}$ [Wbm]) and the anisotropy (MAE [eV], easy axis, and hard axis) are presented.

Density functional theory–based first-principles calculations were performed using the Vienna Ab initio Simulation Package (VASP).[1)] The optimized structures of the bcc-Fe, fcc-Ni, and hcp-Co are shown in Figs. 1(a), 1(b), and 1(c), respectively. Here, a generalized gradient approximation with a PBE type exchange correlation functional was utilized. The wave function was represented by a plane wave basis set with a cutoff energy of 550 eV, and the k-points mesh was set to 16 × 16 × 16 for Fe and Ni, and 16 × 16 × 10 for Co. While calculating the MAE, the convergence conditions for the self-consistent field method were 10^{-9} eV for Fe and Co and 10^{-10} eV for Ni. The spin–orbit interaction was also considered.

The MAE [eV] is generally defined as the difference between the energy in the hard-axis direction and that in the easy-axis direction. In this study, the MAE was calculated as $E_{111}-E_{001}$ for Fe, $E_{001}-E_{111}$ for Ni, and $E_{0001}-E_{2\bar{1}\bar{1}0}$ for Co. Table 1 shows the calculation results of the magnetic moment and the MAE of Fe, Ni, and Co. From this, we find that the magnetic moments agree with the experimental results. The MAE of Fe is greater than the experimental result, and that of Co is less than the experimental result, which are the same in terms of the order of magnitude. Furthermore, the easy axes of Fe and Co agree with the experimental results. In contrast, the MAE of Ni differs from the experimental results in terms of the sign. In other words, the [100] direction is the easy axis and the [111] direction is the hard axis.

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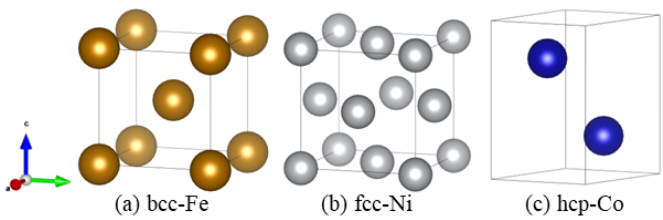

Fig. 1 The optimized structures of the bcc-Fe, fcc-Ni, and hcp-Co

Table 1 Magnetic moment and MAE of Fe, Ni, Co.

	μ [μ_B/atom]		MAE [eV]	
	Calc.	Exp.	Calc.	Exp. [2)]
Fe	2.20	2.20	5.15×10^{-6}	1.99×10^{-6}
Ni	1.60	1.60	8.91×10^{-6}	-4.84×10^{-7}
Co	0.63	0.60	1.41×10^{-5}	8.21×10^{-5}

$\mu_B = 1.165 \times 10^{-29}$ [Wbm]

Magnetoelastic Interaction Modeling of Polycrystalline Magnetic Materials

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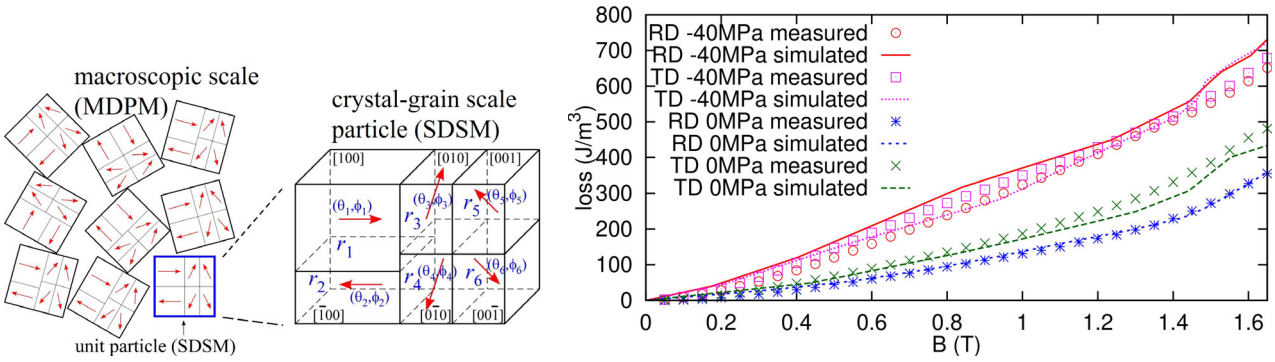
The development of highly efficient electric machines e.g. motors has been required in these days. Because the energy loss of iron-core material can increase under the mechanical stress, several magnetization models have been proposed to represent the stress dependence of magnetizaion properties of iron-core materials. Most of those are phenomenological models, which require measured data to determine their model parameters. However, it is often difficult to measure magnetic properties under a wide range of operational conditions. A physical magnetization model is accordingly required to predict the stress-dependent properties only from basic material constants without using measured data.

One of the difficulties in constructing a physical model is the polycrystalline nature of iron core materials. Taking account of the polycrystalline nature, we have developed a multiscale physical model, called multi-domain particle model (MDPM) to represent the macroscopic magnetization property based on the energy minimization. The MDPM successfully predicted the stress-dependent magnetization properties from material constants without using measured data under the mechanical stress.

The MDPM consists of an assembly of multi-domain particles [Fig. 1(a)]. The magnetization state in a particle is represented by the volume ratios and the magnetization directions of magnetic domains, which are determined by locally minimizing the total magnetic energy consisting of the Zeeman, anisotropy, magnetostatic, and magnetoelastic energies. The variation in the volume ratio is resisted by a pinning field, which causes the hysteresis loss.

The hysteresis loss of non-oriented silicon steel sheet 50A470 was measured and simulated with and without compressive stress of 40 MPa [Fig. 1(b)]. The hysteresis loss increases with the compressive stress significantly. The difference in the loss property between the rolling direction (RD) and transverse direction (TD) decreases under compressive stress. Using an anisotropic pinning field, the MDPM accurately predicts the stress-dependence of hysteresis loss.



(a) multi-domain particle model (b) hysteresis loss per cycle with/without mechanical stress

Fig. 1. Stress-dependent magnetization property simulation using MDPM

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Analytical modeling of Litz wire copper loss for high-frequency high-efficiency power magnetic device design

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Recently, the miniaturization of power supply circuits has been achieved by the high-frequency operation of switching power converters owing to the high-speed switching performance of recent switching devices. However, the high-frequency operation increases the power loss in the power magnetic devices, such as power transformers and inductors, which are emerging as obstacles to further miniaturization.

The power loss of the power magnetic devices can be classified into iron and copper losses. As both losses increase due to the high-frequency operation, intensive research is performed targeting these two losses. However, unlike the reduction of the iron loss, the reduction of the copper loss is difficult to be achieved through material development, because little possibility can be expected to find a material that replaces the copper. Therefore, a reduction of the copper loss should be done by optimizing the wire structure.

Particularly, the Litz wire has been widely utilized for high-frequency applications. The Litz wire is made of many thin copper strands twisted in multiple levels, as illustrated in Fig. 1. The strands are twisted so that each strand equally experiences every position in the Litz wire cross-section, which mitigates the eddy current generation inside the Litz wire and reduce the copper loss in the high-frequency operation. Because of this simple mechanism, only the strand diameter has been long regarded to mainly affect the copper loss characteristics. However, a recent study [1] revealed that the eddy current suppression characteristics can significantly deteriorate in large-diameter Litz wires when compared among the Litz wires with the same strand diameter, as shown in Fig. 2. This indicates that the detailed optimal design should be sought depending on the specifications of the Litz wire.

The copper loss prediction of the Litz wire has long been performed on the FEM analysis [2]. However, in recent high-frequency and high-power applications, the Litz wire needs to twist more than 1000 strands with a diameter of less than 40μm. Due to its complicated structure, the optimal design of Litz wire has been practically difficult to be analyzed and sought by FEM analysis.

To overcome this difficulty, the authors investigated the analytical copper loss modeling of the Litz wire and succeeded to propose a fully analytical copper loss model made only of physical constants and physically measurable parameters of the Litz wire [3]. With the help of this model, the deterioration mechanism of the eddy current suppression characteristics in large-diameter Litz wire was elucidated. This presentation aims to give a full perspective of our current state of study on the analytical copper loss modeling of the Litz wire as well as the usefulness of the Litz wire design through analyzing the deterioration mechanism of the copper loss suppression effect in large-diameter Litz wire.

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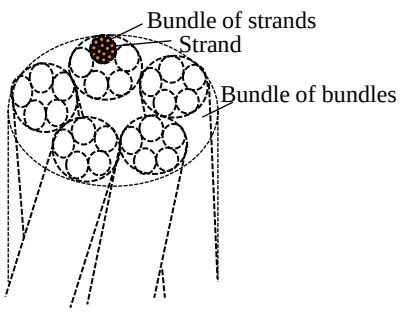

Fig. 1 Multi-level twisting structure of Litz wire.

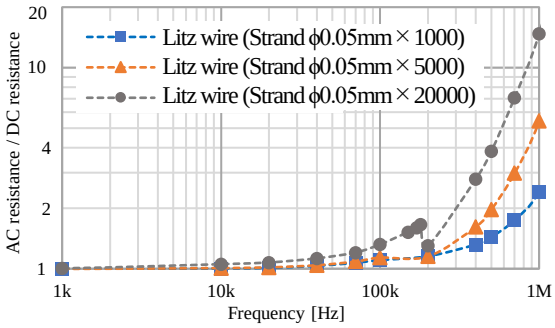

Fig. 2 Measured ratio of ac/dc resistance of Litz wires of same strand diameter.

Quasi-static electromagnetic eddy current analysis based on Darwin model considering both inductance and capacitance effects

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In recent years, advances in SiC and GaN have led to an increasing trend toward higher frequencies in power electronics devices. High frequency inductors, transformers, and capacitors are becoming problematic due to the effects of parasitic capacitance and parasitic inductance as the inverter carrier frequency and drive frequency become higher. Specifically, the increase in equivalent resistance due to the skin effect inside conductors caused by high frequencies, coupling due to magnetic fields and stray capacitance between neighboring conductors, and so on. Although these effects can be determined by measurement, As a countermeasure, it is desirable to utilize electromagnetic field analysis that does not require prototyping. Conventional quasi-magnetostatic field analysis is capable of frequency-domain and time-domain electromagnetic field analysis that takes into account eddy currents and nonlinear magnetic properties of magnetic materials, but it cannot handle dielectrics because its formulation neglects displacement currents. On the other hand, the Darwin model, which has been attracting attention in recent years, can also take quasi-electrostatic fields into account, so it can be applied from low frequencies to the frequency range where electromagnetic waves do not occur.

We have been developed new types of the A-ϕ formulations of the finite element method in the frequency-domain and time-domain 1),2). The methods achieve the low-frequency stability at low frequencies by taking into account the Coulomb-type gauge condition. The two types of the methods have been developed: one without additional variables and one that defines redundant variables to improve convergence characteristics in high-frequency range. The matrix equations can be symmetric. In addition, the method can also handle nonlinear magnetic material properties and coupling electric circuit as well as conventional quasi-magnetostatic analysis.

Fig. 1 shows the analysis model of the gapped core inductor model in which a coil of solid strands doubly wound in a solenoidal shape is wound around a gapped core is used to analyze the effect of parasitic capacitance between the strands. A 1 mm diameter strand of wire elongated from the mesh boundary was helically wound 20 turns from the bottom right to the top on a 10 mm diameter core, and then 20.5 turns were wound from the outside to the bottom, shifting half a pitch of the radius, to the bottom left, extending to the mesh boundary. The conductivity of the conductor was set to 5.e7S/m. The relative permittivity of all components was set to 1. The core was given a relative permeability of 1500 as ferrite, and a 1 mm gap is provided in the center of the coil interior. Fig. 2 shows the electric density distribution at 85kHz solved by frequency-domain analysis. Apparently, it can be seen that a large electric field is generated between the inner and outer strands, especially at the bottom of the coil where the winding starts and ends.

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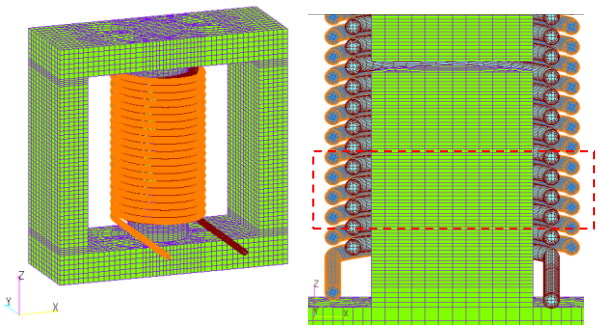

(a) Full model (b) Cross-sectional view

Fig. 1. Gapped core inductor model.

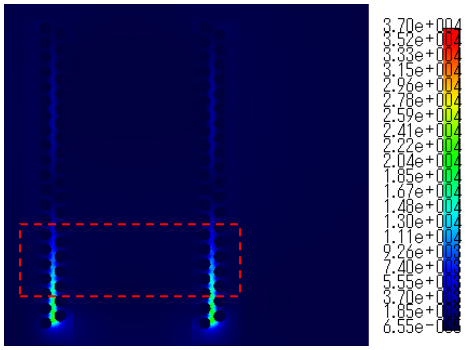

Fig. 2. Electric density distribution at 85kHz.