Rigorous Modeling of Microwave Devices on Magnetic Opal Nanocomposites by the Method of Multimode Autonomous Blocks

G. S. MAKEEVA¹, O.A. GOLOVANOV¹, A.B. RINKEVICH², AND G.A. KOUZAEV³
¹Penza State University, Penza, Russia
radiotech@pnzgu.ru
²Institute of Metal Physics Ural Division of the Russian Academy of Science,
18 Sofia Kovalevskaya St., Ekaterinburg 620041 Russia
rin@imp.uran.ru
³Norwegian University of Science and Technology - NTNU Trondheim, Norway, No-7491, guennadi.kouzaev@iet.ntnu.no

Abstract — A numerical approach for the 3D diffraction boundary problems and for simulation of microwave magnetic nanostructure devices is developed. This numerical technique is based on the solution of the Maxwell equations with electromagnetic boundary conditions complemented by the Landau-Lifshitz equation with the exchange term. The modelled area of magnetic opal nanocomposite is divided into a number of autonomous blocks with magnetic nanoinclusions (MFABs) for which the descriptors (S-matrices) are derived. These blocks connected to each other by virtual Floquet channels. Then, the multimodal S-matrix of the modelled whole device is obtained algebraically from the se descriptors of autonomous blocks using the matching conditions on their common boundaries. As an example, the multimode and multichannel S-matrix of a microwave circulator based on opal Ni₀.₇Zn₀.₃Fe₂O₄ nanocomposite is calculated at frequencies 24-30 GHz. For comparison, the results of our full-wave calculations of S-parameters of this circulator are compared with the ones obtained by simplified calculations using the effective permeability and permittivity of nanocomposite inserters.

Key-Words: modelling, microwave, device, magnetic, nanostructure, diffraction, boundary value problem

I. INTRODUCTION

Research and prediction of new physical phenomena and effects in 3D microwave nanostructure devices require new approaches for accurate electromagnetic (EM) modeling based on the full system of the Maxwell equations and the EM boundary conditions.

In the case of magnetic materials, the above equations should be additionally equipped by the Landau-Lifshitz one describing the magnetic phenomena, which leads to the nonlinearity of models. To reduce the simulations, Maxwell equations can be simplified to take into account only the most important effects or to neglect the nonlinearity of ferrites for weak microwave signals.

The second approach is the solution of full-wave 3D diffraction boundary problems and this approach is much more complicated than the first one. Using the results of rigorous mathematical modeling allows to obtain the increased accuracy and adequacy of calculations of practically used waveguides and integrated components.

In this work, a numerical approach for accurate modeling of 3D magnetic nanostructure devices is proposed which is based on the solution of the Maxwell’s equations with the EM boundary conditions complemented by the full Landau-Lifshitz equation taking into account the exchange term to describe the nonlinear effects in magnetic materials. It is applied for simulation of a waveguide circulator containing nanomagnetic inserters.

The methodology uses the decomposition approach [1]. The modelled area is divided into a number of independently analyzed autonomous blocks (ABs) described by their descriptors (scattering matrices) with the following re-composition of them into the S-matrix of a whole device. This approach provides a simple way to assemble a global matrix and to impose the impedance boundary conditions. Due to that, it is possible to model the complex geometries and to make a quick transition from one boundary value problem to another.
For modeling and computer aided design (CAD) of the linear or nonlinear 3D magnetic nanostructure devices, we have created the computing algorithms using the autonomous blocks with the magnetic nanoincludeions (MFABs). They are connected to each other by 6 virtual Floquet channels. The earlier known and used by us ABs were for homogeneous filling. For instance, they are the multimode ABs [2], minimal ABs [3], and universal ABs [4]. All of them were obtained by the solution of Maxwell equations and simplified equations of the magnetic motion.

In contrast to them, the current MFAB descriptors (scattering matrices $S$) are constructed via the simultaneous solution of the Maxwell equations and the Landau–Lifshitz one, and, in the latter, the exchange-interaction field is taken into account.

In this paper, a nonreciprocal device, waveguide circulator, based on 3D magnetic opal nanocomposites are simulated. The nanocomposites consist of closely packed SiO$_2$ spheres (Fig. 1). The voids between these spheres are filled by a magnetic material. Nanocomposites show interesting magnetic properties and intriguing microwave behavior [5]. The EM characteristics of such nanocomposites can be tuned by external DC magnetic field, and these materials can be used for magnetically-controlled attenuators, filters, circulators, phase shifters, absorbers, etc.

II. RIGOROUS EM MATHEMATICAL THEORY FOR MICROWAVE DEVICES BASED ON 3D MAGNETIC NANOCONSTRUCTURES

Our mathematical simulation is based on the solution of the diffraction boundary problems for Maxwell equations regarding to the electric intensity vector $E(r,t)$, magnetic intensity vector $H(r,t)$ and the magnetic induction vector $B(r,t)$ with the equation of motion of the magnetization vector $M(r,t)$:

$$\nabla \times H(r,t) = \varepsilon_0 \frac{\partial E(r,t)}{\partial t} + \sigma(r,t).$$

$$\nabla \times E(r,t) = -\frac{\partial B(r,t)}{\partial t},$$

$$B(r,t) = M(r,t) + \mu_0 H(r,t)$$

equipped additionally by the EM boundary condition equations.

The magnetization vector $M$ is connected to the magnetic field vector $H$ as in the full Landau-Lifshitz theory [6]:

$$\frac{\partial M(r,t)}{\partial t} = -\gamma (M(r,t) \times H(r,t) + H_{ex}(r,t)) + \omega_0 (\chi_0 H(r,t) - M(r,t)), $$

(2)

$$H_{ex}(r,t) = q \nabla^2 M(r,t).$$

(3)

In the above equations, $\varepsilon_0$ is the vacuum absolute dielectric permittivity, $\varepsilon$ is the relative permittivity of material, $\sigma$ is the conductivity, $\mu_0$ is the vacuum permeability, $\gamma$ is the gyromagnetic ratio, $\omega = \alpha \gamma |H_0|$ is the relaxation frequency. In these formulas, $\alpha$ is the damping parameter, $H_0$ is the bias magnetic field, $H_{ex}$ is the exchange field, $\sigma$ is electric conductivity, $\chi_0$ is the static magnetic susceptibility, $q = 2A/\mu_0 M_0$ with $A$ is the exchange constant, and $M_0 = |M_0|$ is the saturation magnetization value.

Using vector algebra, we represent (3) in the form:

$$H_{ex}(r,t) = q \nabla \times M(r,t).$$

(4)

Taking into account $\nabla \cdot M(r,t) = 0$, let’s introduce a new vector function

$$F(r,t) = \nabla \times M(r,t)$$

and write (3) as

$$H_{ex}(r,t) = -q \nabla \times F(r,t).$$

(5)

Representing all these vector functions in the form of series in terms of the combination frequencies $\omega_m$ and substituting these series into (1),(2), and (3) we reduce the nonstationary nonlinear equations to the stationary nonlinear ones at the combination frequencies $\omega_m$.

$$\nabla \times H(\omega_m) = i\omega_m \epsilon_0 \frac{\partial \epsilon(\omega_m) E(\omega_m)}{\partial t},$$

$$\nabla \cdot E(\omega_m) = -i\omega_m M(\omega_m) - i\omega_m \mu_0 H(\omega_m),$$

$$\gamma \sum_{j=1}^{\infty} \gamma_j \left( M(\omega_j) \times (H(\omega_j) + H_{ex}(\omega_j)) \right) =$$

$$= -i(\omega_j + i\omega_m) M(\omega_m) +$$

$$+ \omega_0 \chi_0 H(t) - \gamma M_0 \times H(\omega_m) -$$

$$-\gamma M_0 \times H_{ex}(\omega_m) - \gamma M(\omega_m) \times H_0,$$

$$\nabla \times M(\omega_m) = F(\omega_m),$$

$$\nabla \times F(\omega_m) = -q^{-1} H_{ex}(\omega_m).$$

In (7), \( \omega_m > 0, \omega_{-m} = -\omega_m, \omega_0 = 0 \) for $m = \pm 1, \pm 2, \ldots$ .

Additionally,
\[ \dot{e}(\omega_m) = c(\omega_m) - i \frac{\sigma(\omega_m)}{\varepsilon_0 \omega_m}, \] with \( i \) as the imaginary unit,
\[ M_0 = M(\omega_0). \]

\[ \gamma_{jk} = \begin{cases} 
0, & \text{if } \omega_j + \omega_k \neq \omega_m \\
1, & \text{if } \omega_j + \omega_k = \omega_m 
\end{cases}. \]

III. NUMERICAL APPROACH USING AUTONOMOUS BLOCKS WITH THE FLOQUET CHANNELS

As was mentioned, the MFAB scattering matrix is obtained by solving the 3D diffraction boundary problem for the Maxwell and Landau-Lifshitz equations with the EM boundary conditions.

The 3D magnetic opal nanocomposite is divided into a number of autonomous blocks (Fig. 1a) in the form of a rectangular parallelepiped containing opal nanoparticles and magnetic material filling the void regions. These blocks are connected to each other with virtual Floquet channels on the block’s bounds (input sections \( S_\alpha \) ) (Fig. 1b).

![Fig. 1. Separation of a 3D magnetic opal piece into a number of autonomous blocks: a - 1 - region, filled by magnetic nanoparticles; 2 - SiO2 nanospheres; b - autonomous block in the form of a rectangular parallelepiped with virtual Floquet channels: \( V_0 \) is the basic region; \( V = V_0 \cup V_1 \cup V_2 \cup V_3 \) are regions of dielectric nanospheres; \( V_a \) is the region of magnetic nanoparticles; \( a, z_a (\alpha = 1,2,...,6) \) are local coordinate systems on input sections \( S_\alpha \) (bounds).](image)

We consider the MFAB as a “waveguide transformer” with its descriptor as a multimode multi-channel scattering matrix \( EM \) obtained taking into account the boundary conditions.

We use the eigenwaves of the rectangular cavity (Fig. 1b) as the basic functions \( \{ E_{n(m)} \}, \{ H_{n(m)} \} \), where \( n \) is the index of a basis function and \( m \) is the index of a combination frequency. We determine the eigenfrequencies \( \omega_m \) and the eigenwaves \( \{ E_{n(m)} \}, \{ H_{n(m)} \} \) by solving the homogenous Maxwell’s equations with the periodic boundary conditions on the walls of the rectangular cavity (the MFAB bounds) (see Fig. 1b).

We find the solution of the diffraction problem for the stationary nonlinear equations (7) with the non-asymptotic radiation boundary conditions [7] in the form of Fourier’s series using the electric and magnetic field eigenmodes \( \{ E_{n(m)} \}, \{ H_{n(m)} \} \) of the rectangular cavity inside the MFAB region \( V_0 \) (Fig. 1b) or eigenwaves \( \{ e_{l(\beta)}(\omega_m) \}, \{ h_{l(\beta)}(\omega_m) \} \) of Floquet channels on MFAB input cross-sections (Fig. 1b).

The tangential EM field on each MFAB input cross-section is represented as a superposition of eigenwaves of Floquet channels [4]:

\[ E_{(\beta)}(\omega_m) = \sum_{l=1}^{\infty} \left( c_{l(\beta)}^+(\omega_m) + c_{l(\beta)}^-(\omega_m) \right) E_{l(\beta)}(\omega_m), \]
\[ H_{(\beta)}(\omega_m) = \sum_{l=1}^{\infty} \left( c_{l(\beta)}^+(\omega_m) - c_{l(\beta)}^-(\omega_m) \right) H_{l(\beta)}(\omega_m), \]

where \( C_{l(\beta)}^+(\omega_m), C_{l(\beta)}^-(\omega_m) \) are the magnitudes of the incident and reflected modes, \( \beta \) is the index of a MFAB cross-section, \( l \) is the index of an eigenwave. We find the unknown magnitudes \( C_{l(\beta)}^-(\omega_m) \) of the reflected modes when the magnitudes \( C_{l(\beta)}^+(\omega_m) \) of the modes incident on the MFAB input cross-sections are regarded to be known.

Substituting the Fourier’s series (8) into the stationary nonlinear equations (7), which are represented at projecting integral form [8], we obtain the system of nonlinear algebraic equations. These equations are solved using the iterative method from [9] or, alternatively, the Newton’s method described in the same book.

IV. RESULTS OF NUMERICAL SIMULATION OF A 3D NONRECIPOCAL MAGNETIC OPAL NANOCOMPOSITE DEVICE

Let us consider a specific example for a 3D microwave nonreciprocal device. The waveguide circulator (Fig. 2) contains two directional couplers (slot bridges 7) with the insertions of magnetic opal nanocomposite...
(magnetized by the external DC magnetic field $\mathbf{H}_0$ of the antiparallel orientation) 5 in one channel and the dielectric insertions 6 in other channel (Fig. 2).

According to the decomposition approach [1], the region of the waveguide circulator between the sections $S_1$ and $S_2$ (see Fig. 2) is split by the imaginary boundaries (vertical dashed lines) into several sub-regions: two directional couplers 7, four sections of waveguides 8, a waveguide section with the insertions of magnetic opal nanocomposite 5, and a waveguide section with the dielectric insertions 6.

**Fig. 2.** Waveguide circulator based on the 3D magnetic opal nanocomposite: 1, 2, 3, 4 - ports of this circulator, 5 - magnetic nanocomposite insertions, 6 - dielectric ($\epsilon_5=\mu_5=1$) insertions, 7 - directional couplers, 8 - waveguide section, $a=7.2$ mm, $b=3.6$ mm, $c=1.5$ mm, $d=1$ mm, $\Delta=14.4$ mm, $\Delta_i=13.8$ mm, $\delta=24.5$ mm.

The model of the waveguide section with the dielectric insertions was created using the descriptors of universal ABs with Floquet channels [4]. The waveguide sections with the magnetic nano-material are modeled with the help of MFABs which are described by multimode multi-channel S-matrices with the elements $R_{k\alpha}$ ($\alpha, \beta$ are the numbers of the input cross-sections; $k,n=1,2,...$ are the indices of eigenwaves of waveguide).

The second model of the waveguide circulator was created using the calculated values of the effective EM parameters of 3D opal magnetic nanocomposite, and it is simplified one for comparison with our full-wave simulations. For calculations of complex diagonal $\mu^x$ and off-diagonal $\mu^v_{\alpha}$ components of this effective permeability tensor and the effective permittivity $\epsilon^x$ of 3D opal magnetic nanocomposite, the EM model from [10] was used. There, a cell is described by its MFAB conductivity matrix $\hat{\mathbf{Y}}$ taking into account the EM boundary conditions and the number of ferromagnetic particles $N$ filling the octahedral opal void regions (Fig. 1b) in each cell.

Using MFABs, the results of calculation of the complex scattering parameter $R_{11}^{12}=R_{11}^{12}\exp(i\phi^{12})$ and $R_{11}^{21}=R_{11}^{21}\exp(i\phi^{21})$ of the S-matrix of the rectangular waveguide section with the magnetic nanocomposite insertions (Fig. 2) depending on the DC magnetic field $H_0=\mathbf{H}_0$ at $f=30$ GHz are shown in Fig. 3. The difference $\phi^{21}-\phi^{12}$ between the phases of the forward and backward $10_{TE}$ modes propagating in this waveguide section is equal to $\phi=\phi^{21}\Big|_{H_0=9.8\text{ kOe}} = 5.88\pi$ (Fig. 3).

**Fig. 3.** Reflection coefficient magnitudes $|R_{11}^{12}|$, $|R_{11}^{21}|$ and their phase arguments $\phi^{12}$, $\phi^{21}$ of a waveguide section with magnetic nanocomposite insertions versus the DC magnetic field $H_0=9.8$ kOe.

The results of calculations of the modulus of scattering parameters $|R_{11}^{0\phi}|$ of S-matrix of this waveguide circulator, i.e. the transmission coefficients $k_{\alpha\beta}$ of fundamental mode $10_{TE}$ (with magnitude $c^+_{\alpha}$) from the port number $\alpha$ ($\alpha=1,2,...,4$) to the port number $\beta$ ($\beta=1,2,...,4$) depending on the frequency for the DC magnetic field $H_0=9.8$ kOe are shown in Fig. 4 (curves 1-3) for different numbers $N=1,4,8$ of the ferromagnetic nanoparticles with the diameter...
The following parameters were used in the calculations: the radius of the SiO$_2$ nanospheres $r_{nm} = 100$ nm. For magnetic nanoparticles Ni$_{0.7}$Zn$_{0.3}$Fe$_2$O$_4$ with $4\pi M_s = 5$ kG, the exchange constant $A = 2.2 \times 10^{-9}$ Oe cm$^2$, the damping parameter $\alpha = 0.08$, and the relative permittivity $\varepsilon_{mr} = 9.5 - i0.3$.

Fig. 4. Frequency dependences of modulus of the transmission coefficients $k_{\alpha\beta}$ of the TE$_{10}$ wave from the port of number $\alpha (\alpha = 1,2,\ldots,4)$ to the port of number $\beta (\beta = 1,2,\ldots,4)$ of waveguide circulator based on 3D opal magnetic nanocomposite: solid line - rigorous model using MFABs; dashed line - simplified model using the effective parameters; curve 1 - $N = 1$, $d = 50$ nm; curve 2 - $N = 4$, $d = 35$ nm; curve 3 - $N = 5$, $d = 25$ nm; $H_0 = 9.8$ kOe.

The results of rigorous modeling by MFAB method (solid lines in Fig. 4) are compared with the results of simplified calculations (dashed lines in Fig. 4). It is seen increasing difference with the number of magnetic nanoparticles filled the void regions.

This numerical method and developed computational algorithms can be used to simulate the 3D microwave devices based on magnetic nanostructures of arbitrary shapes. They are to investigate and predict new physical phenomena and new effects in the nano-based devices, which can be used to enhance many microwave passive devices and systems [11].

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References