# Modeling of Magnetodielectric Effects in Magnetostrictive/Piezoelectric Multi-layers Using a Multiphysics Simulator.

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**Abstract:** In this paper, we use COMSOL, finite element software, to compute the magnetodielectric effect in a multiferroic structure based on a {ferromagnetic / piezoelectric} multi-layer. We also investigate the potential tunable applications of such structures at microwave frequencies. In a first part, we present the piezoelectric and magnetostrictive equations which were then used to develop the global magnetodielectric model. To validate the magnetostrictive model, results of simulation were then compared to published experimental results. The global magnetodielectric model was also validated using microwave measurements of a FeCoB / PVDF / FeCoB tri-layer structure. Finally, we associated magnetodielectric and RF models to investigate the potential of different structures to tunable microwave applications.

**Keywords:** Finite elements, Magnetodielectric effect, Magnetostriction, Mechanics, Piezoelectricity, RF tunable circuits.

## 1. Introduction

The integration of several services in wireless terminals is a burning issue for industrials. Indeed, each service is associated with a standard corresponding to an own frequency band: GSM (900-1800MHz) for the telephony, Wi-Fi (2.4-2.48GHz) for internet... Thus, each service requires the implementation of its own RF circuits leading to an increase of cost, weight and power consumption. To overcome this issue, a solution consists in using tunable microwave devices

Since a few years, several technological ways (semiconductors, ferroelectrics, ferromagnetics, liquid crystals, MEMS …) were investigated by industrials and laboratories to realize such tunable devices. An alternative way consists in using composite materials which exhibit multiferroic properties. Using these materials, a variation of permittivity and/or permeability can be considered through the application of an electric field. Indeed, the magnetodielectric effect, considered in such materials, is a combination between magnetostrictive and piezoelectric effects. The application of an electric field to the piezoelectric layer will lead to the creation of an induced magnetic field in the magnetostrictive material thanks to mechanical couplings.

$$magnetodielectric = \frac{magnetic}{mechanic} \times \frac{mechanic}{electric} \quad (1)$$

$$magnetodielectric = magnetostriction \times piezoelectricity \quad (2)$$

The design of a new generation of smart systems using this effect needs models in order to optimize efficiently such structures.

We chose to implement our modeling by using Comsol Multiphysics software which is a very user-friendly environment enabling the simulation of multiphysics problems. A piezoelectric model is integrated in Comsol. We developed a magnetostrictive model which enabled us to evaluate the magnetic field induced in a magnetic material by a mechanical stress. The association of these models enabled us to simulate a static magnetodielectric effect. Finally, combining the magnetodielectric model with the RF one allowed us to evaluate the potential of magnetodielectric structure at microwave frequencies (Fig. 1).

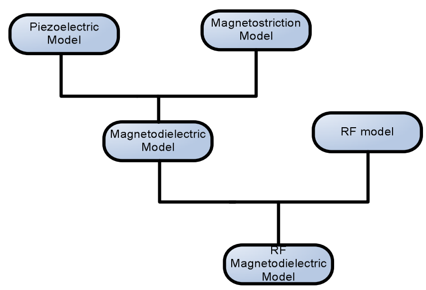


**Figure 1**. Schematic description of the constitutive builded model in this work.

In this paper, we firstly introduce the equations which were used to develop the magnetostrictive model and the global magnetodielectric one. In a second part, these models are validated by comparing the results got using Comsol Multiphysics with static experimental results. Finally, we associated the developed magnetodielectric model to the RF one in order to evaluate the potential of different structures to microwave tunable applications.

## 2. Thermodynamic approach for the formulation of magnetodielectric equation

### 1.1 Piezoelectric equations

Using the first law of thermodynamic, the internal energy of an electromechanical system can be expressed as:

$$dU = \sigma_{ij} dS_{ij} + E_i dD_i + Td\Theta \qquad (3)$$

Where $\sigma_{ij}$, $S_{ij}$, $E_i$, $D_i$, U, Θ, and T correspond respectively to the stress, strain, electric field, electric displacement, internal energy, the entropy, and the temperature.

The Gibbs free energy is defining as:

$$G = U - E_i D_i - T\Theta \qquad (4)$$

The total differential of G gives us:

$$dG = \sigma_{ij} dS_{ij} - D_i dE_i - \Theta d\delta T \qquad (5)$$

This last equation can also be written:

$$\sigma_{ij} = \left(\frac{\partial G}{\partial S_{ij}}\right)_{E,T}, D_i = -\left(\frac{\partial G}{\partial E_i}\right)_{S,T}, \Theta = -\left(\frac{\partial G}{\partial \delta T}\right)_{S,E} \qquad (6)$$

A second derivation gives us Maxwell-Callen's relationships:

$$\left(\frac{\partial \sigma_{ij}}{\partial E_m}\right)_{S,T} = -\left(\frac{\partial D_m}{\partial S_{ij}}\right)_{E,T}, \left(\frac{\partial \sigma_{ij}}{\partial \delta T}\right)_{S,E} = -\left(\frac{\partial \Theta}{\partial S_{ij}}\right)_{E,T} \qquad (7)$$

$$\left(\frac{\partial D_m}{\partial \delta T}\right)_{S,E} = \left(\frac{\partial \Theta}{\partial E_m}\right)_{S,T} \qquad (8)$$

These different equalities enable us to establish the relationships between the constants that define the effect of stress on the electrical state and the effect of an electric field on the strain state of the material. We thus obtain nine constants:

$$\frac{\partial \sigma_{ij}}{\partial S_{kl}} = C_{ijkl}, \frac{\partial \sigma_{ij}}{\partial E_n} = -d_{ijn}, \frac{\partial \sigma_{ij}}{\partial \delta T} = -\tau_{ij} \qquad (9)$$

$$\frac{\partial D_n}{\partial S_{kl}} = d_{nkl}, \frac{\partial D_m}{\partial E_n} = \varepsilon_{mn}, \frac{\partial D_m}{\partial \delta T} = \zeta_m \qquad (10)$$

$$\frac{\partial \Theta}{\partial S_{kl}} = \tau_{kl}, \frac{\partial \Theta}{\partial E_n} = \zeta_n, \frac{\partial \Theta}{\partial \delta T} = C_v \qquad (11)$$

Where C, $d_{ijn}$ ($d_{nkl}$), $\zeta_m$ ($\zeta_n$), $\varepsilon_{nm}$ and $C_v$, denote respectively the elastic, piezoelectric, pyroelectric, permittivity tensors, and heat specific.

Considering an adiabatic process, the electro-mechanical expressions are only taken into account. Thus, the piezoelectric equations result in:

$$\sigma_{ij}(E,S) = C_{ijkl}{}^{E} S_{kl} - d_{kij} E_k \qquad (12)$$

$$D_i(E,S) = d_{ikl} S_{kl} + \varepsilon^{S}{}_{ij} E_j \qquad (13)$$

As the finite element software Comsol Multiphysic needs vectorial notation [2], the piezoelectric equation can finally be written:

$$\sigma_I = \sum_{J=1}^{6} C_{IJ}{}^{E} S_J + \sum_{j=1}^{3} E_j d_{iJ} \qquad (14)$$

$$D_i = \sum_{J=1}^{6} d_{iJ} S_J + \sum_{j=1}^{3} \varepsilon_{ij} E_j \qquad (15)$$

With (I, J) Є $A^2$, A= {1, 2...6} and (i, j) Є $B^2$, B= {1, 2, 3}

### 1.2 Magnetostrictive equations

A similar approach to the one used to get piezoelectric equations can be set up to describe the magnetostrictive effect. Using the first law of thermodynamic, the internal energy of a magneto-mechanical system can be expressed as:

$$dU = \sigma_{ij} dS_{ij} + B_i dH_i + Td\Theta \qquad (16)$$

Where $\sigma_{ij}$, $S_{ij}$, $H_i$, $B_i$, U, $\theta$, and T, denotes respectively the stress, strain, magnetic field, magnetic induction, internal energy, the entropy, and the temperature.

The Gibbs free energy is defining as:

$$G = U - H_i B_i - T\Theta \qquad (17)$$

The total differential of G gives us:

$$dG = \sigma_{ij} dS_{ij} - B_i dH_i - \Theta d\delta T \qquad (18)$$

This equation can also be written:

$$\sigma_{ij} = \left(\frac{\partial G}{\partial S_{ij}}\right)_{H,T}, B_i = -\left(\frac{\partial G}{\partial H_i}\right)_{S,T}, \Theta = -\left(\frac{\partial G}{\partial \delta T}\right)_{S,H} \qquad (19)$$

A second derivation gives us Maxwell-Callen's relationships:

$$\left(\frac{\partial \sigma_{ij}}{\partial H_m}\right)_{S,T} = -\left(\frac{\partial B_m}{\partial S_{ij}}\right)_{H,T}, \left(\frac{\partial \sigma_{ij}}{\partial \delta T}\right)_{S,H} = -\left(\frac{\partial \Theta}{\partial S_{ij}}\right)_{H,T} \qquad (20)$$

$$\left(\frac{\partial B_m}{\partial \delta T}\right)_{S,H} = \left(\frac{\partial \Theta}{\partial H_m}\right)_{S,T} \qquad (21)$$

These different equalities can be used to define the constants that establish the relationships between the effect of stress on the electrical state and the effect of an electric field on the strain state of the material:

$$\frac{\partial \sigma_{ij}}{\partial S_{kl}} = C_{ijkl}, \frac{\partial \sigma_{ij}}{\partial H_n} = -q_{ijn}, \frac{\partial \sigma_{ij}}{\partial \delta T} = -\tau_{ij} \qquad (22)$$

$$\frac{\partial B_n}{\partial S_{kl}} = q_{nkl}, \frac{\partial B_m}{\partial H_n} = \mu_{mn}, \frac{\partial B_m}{\partial \delta T} = \zeta_m \qquad (23)$$

$$\frac{\partial \Theta}{\partial S_{kl}} = \tau_{kl}, \frac{\partial \Theta}{\partial H_n} = \zeta_n, \frac{\partial \Theta}{\partial \delta T} = C_v \qquad (24)$$

Where $C_{ijkl}$, $q_{ijn}$ ($q_{nkl}$), $\zeta_m$ ($\zeta_n$), $\mu_{mn}$ and $C_v$, denote respectively the elastic, piezomagnetic, pyromagnetism, permeability tensors, and heat specific.

Considering an adiabatic process, the magneto-mechanical equations can be simplified to:

$$\sigma_{ij}(H, S) = C_{ijkl}{}^{H} S_{kl} - q_{kij} H_k \qquad (25)$$

$$B_i(E, S) = q_{ikl} S_{kl} + \mu^{S}{}_{ij} H_j \qquad (26)$$

As the finite element software Comsol Multiphysic needs vectorial notation [2], the magnetostrictive equations can finally be written:

$$\sigma_I = \sum_{J=1}^{6} C_{IJ}{}^{H} S_J + \sum_{j=1}^{3} H_j q_{iJ} \qquad (27)$$

$$B_i = \sum_{J=1}^{6} q_{iJ} S_J + \sum_{j=1}^{3} \mu_{ij} H_j \qquad (28)$$

With (I, J) Є $A^2$, A= {1, 2...6} and (i, j) Є $B^2$, B= {1, 2, 3}

### 1.3 Magnetodielectric equations

Combining (eq. 14 and eq. 27) piezoelectric and magnetostrictive equations enable us to describe the magnetodielectric effect:

$$\sigma_I = \sum_{J=1}^{6} C_{IJ}{}^{E} S_J + \sum_{j=1}^{3} E_j d_{iJ} \qquad (29)$$

$$\sigma_I = \sum_{J=1}^{6} C_{IJ}{}^{H} S_J + \sum_{j=1}^{3} H_j q_{iJ} \qquad (30)$$

With (I, J) Є $A^2$, A= {1, 2...6} and (i, j) Є $B^2$, B= {1, 2, 3}

The magnetodielectric model was numerically implemented using Comsol Multiphysics.

## 3. Magnetostrictive and magnetodielectric models implementation and validation

The magnetostriction model was firstly implemented using Comsol. To validate this model, we compared Comsol-based simulation results to experimental measurements realized on a Silicon/Terfenol bilayer structure. A schematic view of the considered cantilever structure is presented in figure 2.

The total structure is described thanks to 22500 elements. The simulation results achieved using our implemented magnetostrictive model are presented in figure 3. A deflection of 2.344µm is observed for a 0.05T magnetic field. Figure 4 shows a comparison between the experimental deflections measured on the considered cantilever [3] and the deflection obtained using our modeling. The very similar deflections observed validate our implemented magnetostrictive modeling.

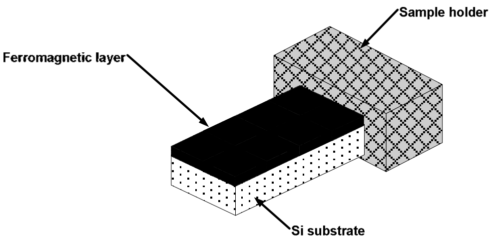


**Figure 2**. Schematic view of a TbDyFe/Si cantilever.

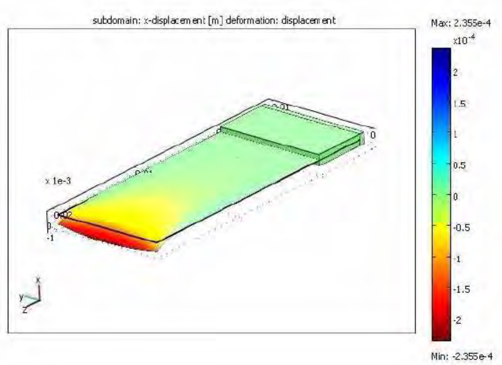

**Figure 3**. Finite-element calculated deflection of a TbDyFe/Si cantilever under a DC magnetic field

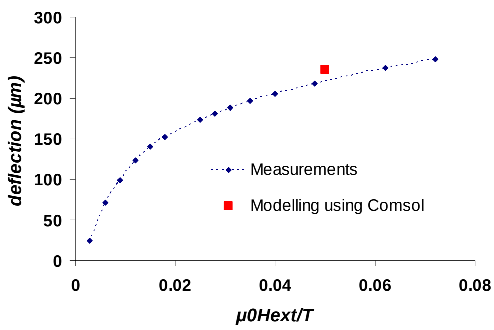


**Figure 4**. Comparison between Comsol-based calculation of the deflection and experimental results for a TbDyFe/Si cantilever.

In a second step, we associated the magnetostrictive model with the piezoelectric model in order to simulate the magnetodielectric effect. A {magnetostrictive / piezoelectric} trilayer structure was selected to test the model. The studied multilayer structure is made up of two 140-nm-thickFigure FeCoB thin films deposited on both faces of a 10-µm-thick PVDF polymer layer.

When an electric field is applied perpendicularly to the plane of the sample (z axis), the inverse piezoelectric effect leads to the creation of a stress in the piezoelectric layer (PVDF). Strains in the polymer layer induce a change in the magnetic anisotropy field of the stressed magnetic layer which modifies its magnetization state and its DC permeability (see Eq. 31).

$$\mu_{DC} = \frac{M_s}{H_a + H_k(V)} \tag{31}$$

When an electric field is applied along the thickness (z axis), the piezoelectric element strain radically leads to inverse piezoelectric effect. The deformation of the polymer induces an equivalent anisotropy field in the strained magnetic layer, which modifies its magnetization state and its permeability.

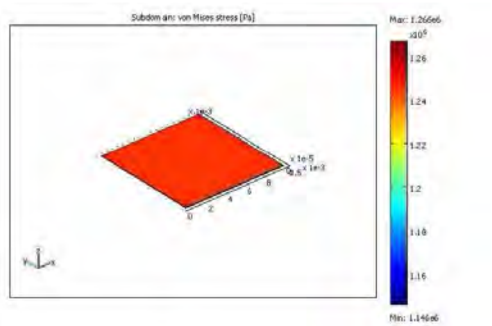

**Figure 5**. State of stress (Pa) in the ferromagnetic layer under a static electric field (U=15V).

Figure 5 presents the state of stress induced in the ferromagnetic layer by the application of a 15V voltage. One should note that the stress induced by the electric field is quite uniform with a mean value of 1.2MPa.

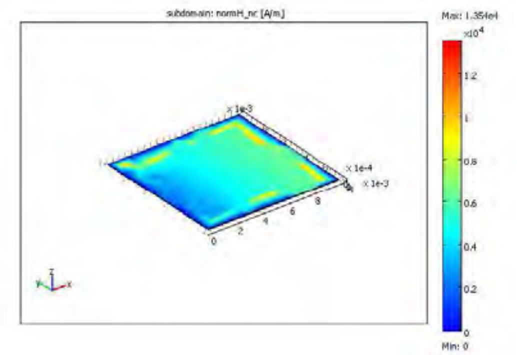


**Figure 6**. Induced magnetic field in the FeCoB layer under a static electric field.

Through mechanical couplings, mechanical stress induced a homogeneous magnetic field of about 60Oe in the ferromagnetic layer (Fig. 6). To validate this FEM-based simulation, we compare these results with experimental measurements [4].

The microwave permeability spectrum of a FeCoB / PVDF / FeCoB trilayer structure was extracted using a single port permeameter [4].

A 30% variation of the microwave permeability (Fig. 6) was observed when a 15V voltage is applied between the two ferromagnetic layers. An additional measurement of the same structure showed very similar variations of the permeability for a 70Oe external magnetic field.

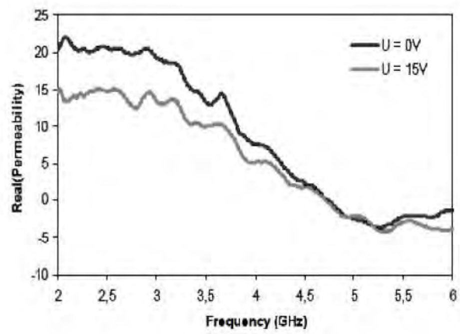


**Figure 7.** Permeability spectrum measured in a tri-layered (FeCoB / PVDF / FeCoB) structure under an electrical voltage U=15V.

Considering that the magnetic field amplitude needed to get similar variations of the permeability than those got using a 15V bias is in the order of the one predicted by our modeling, our magnetodielectric model appears to be sufficiently accurate to simulate such complex structures.

Although the trilayer structure presented before is an interesting structure with a view to validate our modeling, its integration into microwave devices could be complex and difficult to control because of the biaxial nature of the strains induced by the electric field in the piezoelectric layer. However, the validated magnetodielectric model enables us to simulate other complex structures.

Figure 8 presents a chi-type piezoelectric actuator. A magnetostrictive/dielectric multilayer is deposited on the top of the center of the chi actuator. The use of a multilayer structure will enable to increase the interaction between the electromagnetic field and the ferromagnetic materials, as it will be evidenced in section IV. The actuator is constituted of two fixed parts (external boundaries) and its center is mechanically free. The application of an electric field on the fixed parts of the actuator is thus able to create a sufficient uniaxial strain on the center of the structure to change the permeability of the ferromagnetic layers.

Then, the magnetodielectric model was used to evaluate the displacement of the actuator (center part) along the z axis and the induced magnetic field under the action of a 15V voltage (Fig. 8). A displacement of about 1µm along the z axis is thus observed. The stress induced by the application of a 15V bias voltage leads to an induced magnetic field of about 25Oe in the multilayer.

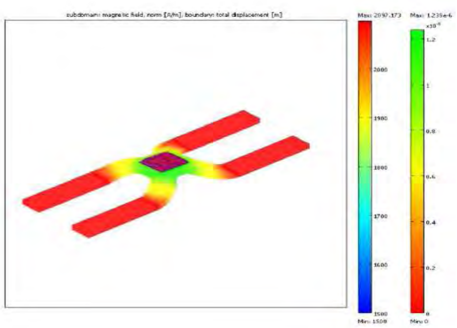

**Figure 8**. Multiphysics simulation of a magnetostrictive/piezoelectric chi-type actuator:

actuator deflection and induced magnetic field in the magnetic core.

## 4. RF simulations of magnetodielectric tunable devices.

In this last section, we combined the magnetodielectric model with the RF one to evaluate the potential of tunable RF functions using Comsol software.

### 4.1 Magnetic tunable stop band filter

Previous investigations at the Lab-STICC laboratory demonstrated the interest of using ferromagnetic/dielectric multilayers in the design of tunable RF devices. A stop-band circuit, constituted of a short-circuited stub loaded by a ferromagnetic/dielectric multilayer, showed thus very interesting tunable properties [5]. Here, we use Comsol software to simulate a similar topology (figure 9). The stub resonator is loaded by a CoFeB/PVDF/CoFeB multilayer (PVDF layers are considered as a simple dielectric material: the magnetodielectric effect is not considered). The application of an external DC magnetic field tends to decrease the permeability of the ferromagnetic layers, and thus, to increase the resonance frequency of the resonator. In order to simulate such effect, the change of permeability under the application of a magnetic field is taken into account by a Kittel law (see Eq. 31), and is considered as an input before computing.

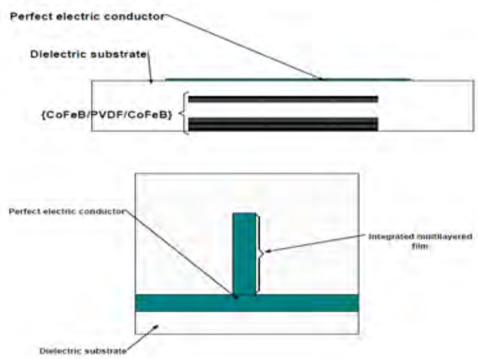


**Figure 9**. Schematic view of a stub resonator loaded by a CoFeB/PVDF/CoFeB multilayer.

Figure 10 shows the transmission parameters of the stub obtained thanks to the RF model of Comsol as a function of frequency and for various DC magnetic fields. By applying a 150Oe magnetic field, a variation of about 8% of the resonance frequency can be achieved: $f_1$ = 1.619GHz and $f_2$ = 1.669GHz. Such tunable devices could be really interesting but the magnetic field bias needs the use of electromagnets whose integration into microwave circuits is difficult. Thus, our interest turned to the electric biasing of such devices.

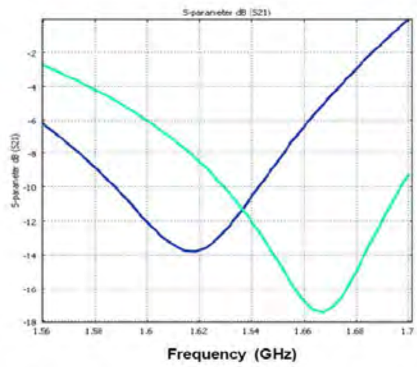


**Figure 10**. Magnitude of simulated transmission coefficient as a function of frequency for various permeability values.

### 4.2 Magnetodielectric tunable microstrip line

Comsol software enables the static modeling of complex magnetodielectric structures such as the chi-type one considered in section 3. In this final part, we associate the chi-type actuator with a microstrip line as shown in Fig. 11. The microstrip line tunablity can be induced by a bias voltage thanks to the magnetodielectric coupling existing between the piezoelectric actuator and the magnetic/dielectric multilayer. The simulation of this complex structure needs the use of “solver manager”. At first, the magnetodielectric model was computed to evaluate the anisotropy field ($H_k$ (V)) induced by a 15V voltage in the ferromagnetic layers (Fig. 11). The variations of the microwave permeability in the ferromagnetic layers are taken into account by applying the Kittel law. Finally, the tensor of permeability can be expressed as:

$$
mu_{RF} = \begin{pmatrix} mu/(H_a+H_k(V)) & 0 & 0 \\ 0 & mu/(H_a+H_k(V)) & 0 \\ 0 & 0 & mu/(H_a+H_k(V)) \end{pmatrix} \quad (32)
$$

Then, the RF model was computed taking thus into account the variations of permeability induced by the bias voltage.

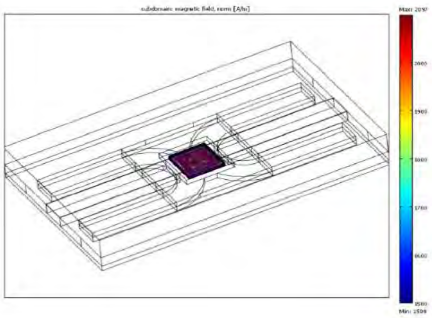

**Figure 11**. Design of microstripe line based on multilayer thick films (Ferro / pvdf / Ferro) and induced magnetic field distribution , actuated by a piezoelectric actuator (uniaxial), driven by an electrical voltage U=15V.

Figure 12 presents the transmission parameter of this loaded microstrip line as a function of frequency for 0V and 15V applied on the piezoelectric actuator. One should note the strong selectivity of the considered resonance. Moreover, by applying a moderate bias voltage (15V), the resonance peak can be tuned of more than 50MHz. Due to its high selectivity; this structure could be notably interesting in the design of tunable microwave oscillators.

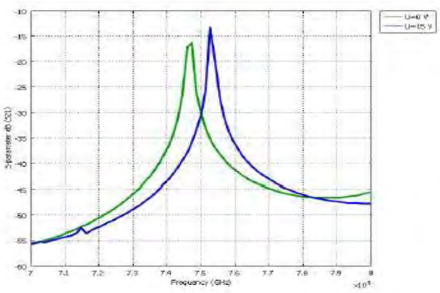

**Figure 12**. Magnitude of the transmission parameter of a microstrip line loaded by a magnetodielectric actuator for 0V and 15V.

## 5. Conclusion and prospect

In this paper, a magnetodielectric model was developed using Comsol Multiphysics by combining a piezoelectric and a magnetostrictive model. This model was validated by comparing simulated and experimental results for a CoFeB/PVDF/CoFeB trilayer. Similar values of anisotropy fields were thus extracted. The association of the developed magnetodielectric model with the RF one enabled us to simulate various magnetodielectric structures and to forecast their potential for tunable microwave applications. Our aim is to soon check these simulation results thanks to experimental measurements of magnetodielectric effect-based tunable microwave devices.

## 6. Références


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