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Implantable NMR Microprobe Design using a Machine learning approach.

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Abstract

In this work, we propose the use of an Artificial Neuronal Network (ANN) to achieve the design process of an implantable Nuclear Magnetic Resonance (NMR) microprobe. Before the micromanufacturing process, we need to optimize the microprobe i.e. micro-coil + transmission line and the connecting path (wire-bonding, underpass&vias or airbridge) to get an optimal performance (high Q -factor and Noise signal Ratio (NSR)). An ANN model is developed from the simulated dataset and used to predict the optimal microprobe performance for a working frequency and the used substrate.

Keywords

Artificial Neural Network, Machine Learning, MSE (mean square error), Matlab, Advanced Design System (ADS) Software, Nuclear Magnetic Resonance Implantable Micro-antenna, 3D-TLE (Transmission Line Extractor).

1 Introduction

One of the main challenges of the Nuclear Magnetic Resonance (NMR) technique is, to improve the sensitivity and spectral resolution in the case of weak metabolites concentration in a small region of interest (ROI $\sim 2\mu\text{L}$ - $3\mu\text{L}$). One way to increase this sensitivity is, to miniaturize the NMR receiver. Thus, the micro-coil part will be adapted to the sample dimension that improves the Signal to Noise Ratio (SNR) performance criteria.

The NMR sensitivity has been the subject of numerous studies for years. Thus, several approaches were already proposed for its optimization: use of higher field [1], and improvement of the sensitivity of the Radio Frequency (RF) coil receiver and transmitter (Microprobe) [2]. In that case, simulation work to optimize the microprobe is required before the manufacturing process. This work remains complex because several parameters must be taken into account to obtain an accurate microprobe Q factor and SNR evaluation (multi-parameters problem). It requires the use of several software, a long computational time. Nowadays artificial intelligence (AI) has been widely used in several application areas, more particularly artificial neural networks (ANN). Recently, they have been used to solve complex problems such as antenna parameters

extractions, structural design and data interpretation for radar, and Multiple-Input and Multiple-Output (MIMO) systems [3], also for optimizing the gain and directivity of a microstrip antenna [4]. ANN are extremely useful in modelling problems where the relationship between inputs of the system is not easily modelled. The advantages of ANN assisted antenna modelling system is reducing computational complexity, saving computational time, decreasing the cost compared to traditional computational modelling, and lead to highly accurate data set analysis [5]. All these advantages represent a great asset to deal with the complexity of our microprobe structure design and expected performances optimization [6][7]. ANN approach helps to establish a relationship between several microprobe geometric parameters, material properties and the working frequency with the microprobe performances parameters (resistance R and Q factor). Then, it makes easy the generalization of microprobe optimization problem. In this work, we demonstrate how, ANN succeed predicting the microprobe performances according to its geometrical parameters, material properties and working frequency. Thanks to the microprobe, generated Data from simulations, we proposed an accurate model.

2 Materials and methodology

2.1 Data generation

A trained ANN model requires a large dataset quantity corresponding to inputs data and their target data (outputs). In our case, the microprobe dataset was generated performing a numerical simulation of microprobe Resistance and Q factor

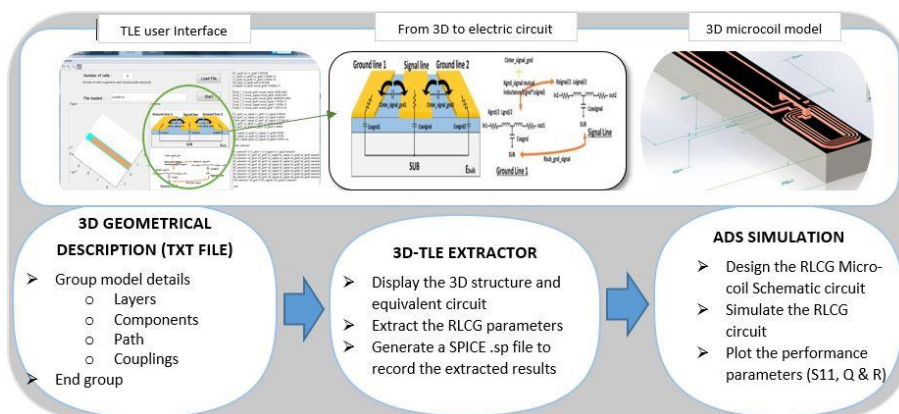


Fig. 1. Block diagrams of the simulation methodology: TLE user interface to 3D micro-coil model

thanks to 3D-TLE (Transmission Line Extractor) platform, and ADS (Advanced Design System) Keysight software. First, we simulated the micro-coil part, where four geometries were designed. Then 3D-TLE, homemade software helped to extract the transmission line electrical parameters and then propose an equivalent electrical circuit of the complete microprobe.

The electrical performances of the microprobe are obtained through the electrical circuit simulated using ADS. By that, we deduce the microprobe resistive losses. Figure 1, summarizes by blocks diagrams the steps from the 3D-TLE platform to ADS software simulations. Thanks to this, we generated 6528 data samples, used for training, validations and test set. The microprobe dataset includes four micro-coil geometries (Rectangular, Ellipsoidal, square and circular), eight working frequency (from 200 MHz to 900 MHz), and two substrate types (glass and silicon).

2.2 ANN Modelling

The Artificial Neuronal Network (ANN) was conceived using the MATLAB Toolbox, Deep Learning (DL). In figure 2, we show the ANN shallow architecture. Note that, between the input layer (Predictors) and the output layer (Targets), there is only one hidden layer that we optimized making trial testing. The data sample was divided into three sets: 70% for training,

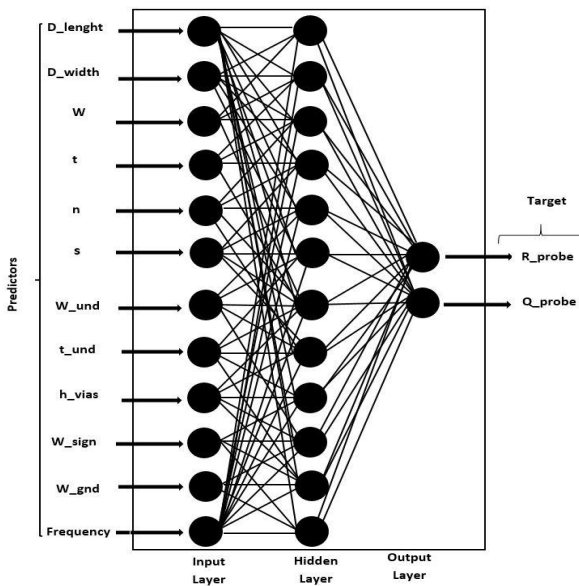


Fig. 2. ANN architecture for Microprobe dataset training model

15% for validation and 15% for test usage. To train our model, we used a custom-made script to automatically test a different number of the neuron from the hidden layer. That script allows choosing the optimal amount of neuron from the hidden layer in terms of MSE (mean square error) Test dataset performance.

3 Results and Conclusions

Figure 3 shows the plot of the microprobe Q-factor from the prediction of the ANN model and the one from the true data value. We can note that the prediction and true data value are in good concordance, which means that we can predict accurately the Q factor of the microprobe, based on its geometrical

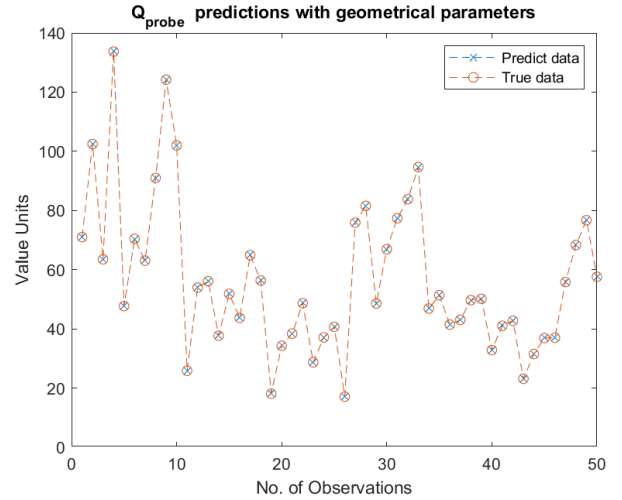


Fig. 3. The microprobe Q factor prediction and the true value

parameters, working frequency and materials properties.

As it is shown, our artificial intelligence algorithms (ANN) were validated to predict well (RMSE = 0.0316 Test dataset), the Q - factor of the microprobe even for a dataset of 6528 samples, which correspond to 99.8% for accuracy of the model prediction in term of to the Test performance.

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