

Modeling LSPR Nano-particles by Using Neural Networks

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ABSTRACT

Localized surface plasmon resonance (LSPR) biosensors represent a relatively new and hot research topic in biosensing applications. Since the fabrication of LSPR biosensors is time consuming and costly, providing a mathematical model that can predict the LSPR characteristics before any fabrication is on edge. Implementing such a model for the LSPR devices, and then optimally designing the LSPR geometrical parameters for a particular surface enhanced Raman Scattering (SERS) biosensor function is the concept that has not been explored yet. In this paper, a multi layered artificial neural network (ANN) is proposed which produces a mathematical model representing the characteristics of LSPR devices as a function of their physical dimensions for a specific shape of nano-particles. Such a model can be used to identify a LSPR structure that is appropriate for a biosensing application requiring specific LSPR characteristics. The numerical electromagnetic modeling approach of the finite difference time domain (FDTD) method, and the analytical method of electrostatic eigenmode are used to implement the proposed model.

Categories and Subject Descriptors

F. [Theory of Computation]: Models of Computation - *Self-modifying machines (e.g., neural networks)*.

F.2 [Analysis of Algorithms and problem Complexity]: Numerical Algorithms and Problems – *Computations in finite fields*.

G.1 [Numerical Analysis]: Numerical Linear Algebra – *Eigenvalues and eigenvectors (direct and iterative methods)*. Optimization - Ordinary Differential Equations – *Finite difference methods*.

General Terms

Algorithms, Design, Theory.

Keywords

Artificial neural network, optimization, localized surface plasmon resonance, numerical method.

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1. INTRODUCTION

Localized surface plasmon resonance (LSPR) devices have a wide range of applications in Raman biosensors, solar cells, DNA rulers and others. In particular, for the Raman biosensor application, the amplitude of the scattered wave is usually very small, making measurement quite challenging.

A potential method to increase the sensitivity of surface enhanced Raman scattering (SERS) biosensors consists of magnifying the incident wave by using noble metal nano-particles (NPs) of size and shape that guarantee enlarged plasmon resonances on the surface of the nano-particles in the desired wavelength range. The enhanced electric field which is localized around the NPs is due to the LSPR phenomenon. The phenomenon happens when light interacts with noble NPs at their resonance wavelength. Noble metals are used in LSPR because their permittivity at the visible-Near Infra-red wavelength range is complex and exhibit negative real part. Such condition is mandatory for generating surface plasmons. The resonance spectrum is a function of the NP shapes, physical dimensions, substrate, and light polarization [1-5].

Moreover, if the resonators present sharp discontinuities, e.g. tips, gaps, etc., the electric field near such discontinuities diverges, and a significant increase of its amplitude is obtained. The authors of the present publication have previously proposed nano-sinusoid NPs which have shown more enhanced electric field with more linearity as a function of the size of the NPs than other sharp tip NPs like nano-triangles, and nano-diamonds (see Figure 1) [6].

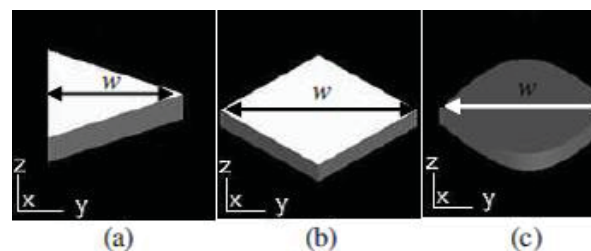


Figure 1. (a) Nano-triangle, (b) nano-diamond, and (c) nano-sinusoid.

Also, it has been shown that using NPs in a 1D array configuration can significantly increase the electric field enhancement in the space between the NPs which are called hot spots (see Figure 2) [7].

Finding a numerical model to predict the LSPR spectrum before timely and costly fabrication of the device is essential which has

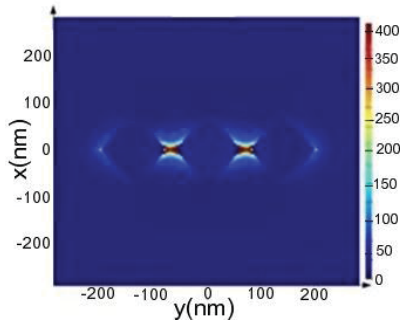


Figure 2. Enhanced electric field (hot spots) between nano-sinusoid NPs

been only marginally considered. In this paper, an artificial neural network (ANN) is developed to model formulas representing the characteristics of LSPR devices as a function of their geometrical parameters. Using the trained ANN architecture, the behavior of LSPR devices for a given set of physical dimensions can be predicted. This model is appropriate for a particular biosensing application requiring specific LSPR spectrum characteristics. The statistical technique of response surface method (RSM) [8] is used to design the minimum required physical data sets for the simulation process, guaranteeing the stability of the developed ANN model. Furthermore, the numerical electromagnetic modeling approaches of the finite difference time domain (FDTD) method [9] and the analytical method of electrostatic eigenmode [10, 11] are used to implement the proposed method.

2. PRINCIPLE OF OPERATION

The proposed procedure for modeling the LSPR biosensors, shown in Figure 3, includes the following steps:

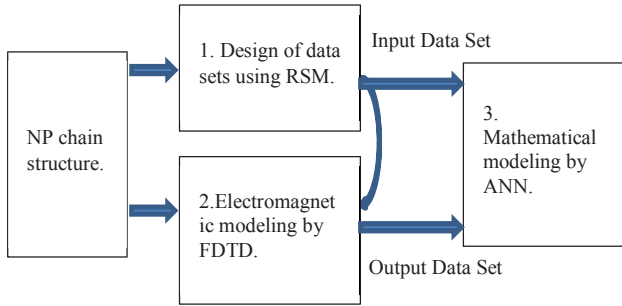


Figure 3. Flowchart of the modelling and optimization procedure.

1. *Design of Input Data Sets:*

To model the LSPR behavior using ANN with the least residual error, first the best input data sets are designed using the RSM software. In this step, the input values of the required simulations are designed and stated in the first four columns of Table 1 (green coloured columns). RSM calculates the total number of input data sets and the values of each set. The physical dimensions of the NPs, including NP in-plane width, height, number of NPs in each array, and

Table 1. Input/out data sets.

Thickness (nm)	Width (nm)	Spacing (nm)	Chain no.	Extinction Cross section (nr ²)	Resonance Wavelength (nm)	FWHM (nm)
Input Data Set 1 designed by RSM (1 st step)				Output Data Set 1 resulted from Electromagnetic Modeling (3 rd step)		
.				.		
.				.		
.				.		
Input Data Set n designed by RSM (1 st step)				Output Data Set n resulted from Electromagnetic Modeling (3 rd step)		

the spacing between the NPs are elements of each data set. The range of these data is taken as follows:

$$\begin{aligned}
 10 &\leq h = \text{Thickness (nm)} \leq 40 \\
 80 &\leq w = \text{in-plane width (nm)} \leq 150 \\
 5 &\leq s = \text{Spacing (nm)} \leq 45 \\
 2 &\leq l = \text{Chain_no} \leq 5
 \end{aligned}$$

According to the range of these elements, RSM finds the optimum number of data sets and their values.

2. *Electromagnetic Modelling:*

Maxwell's equations describing the evolution of the electromagnetic field can be solved using both analytical and numerical methods. Since analytic solution of the equations is possible only for some specific geometries, for general shapes numerical methods such as FDTD method is often employed. In [9] this formulation was used to obtain the characteristics of the LSPR. Moreover, the results of the FDTD method is validated by the analytical electrostatic eigenmode method [10,11]. This combined method formulates the plasmon resonance wavelength of a single NP by:

$$\varepsilon_m(\lambda_r) = \varepsilon_b \frac{1+\gamma}{1-\gamma} \quad (1)$$

where λ_r is the LSPR resonance wavelength, $\varepsilon_m(\lambda_r)$ is the permittivity of the metal at the resonance wavelength, ε_b is the dielectric constant of the background media, and γ is the eigenvalue of a single NP. For example, for the dipolar resonant condition for nano-spheres in dipolar mode ($\gamma = 3$) and in a limited range of size Eq. (1) gives $\varepsilon_m(\lambda_r) = -2\varepsilon_b$.

The LSPR spectrum characteristics, including extinction cross section (cr), resonance wavelength (λ), and full width at half maximum (FWHM) are calculated using the FDTD method, as shown in Table 1.

3. Mathematical modelling by the ANN:

The architecture of the ANN used in this work is shown in Figure 4. It has one input layer with four inputs, one hidden layer with 20 nodes, and one output layer with three outputs.

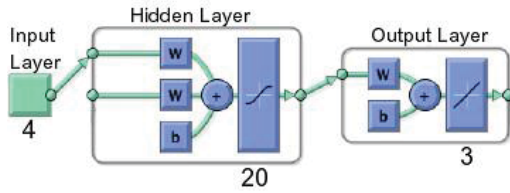


Fig. 4. The ANN configuration.

The ANN builds models on the input/output (*Thickness, in-plane width, Spacing, Chain no / Extinction Cross Section, Resonance Wavelength, FWHM*) data sets denoted in Table 1. In the ANN, the relationships between the input- and the output-data are determined by the ANN coefficients.

However, it should be mentioned, that the considered method presents the usual limitations of any ANN based solution.

3. SIMULATION RESULTS AND DISCUSSION

The input data suggested by RSM software is applied to the FDTD modeling program. Based on each input data set, one set of output data is generated by the FDTD model. The input/output set is applied to the ANN as training data sets. The input/output set is applied to the ANN as training data sets. The minimum number of sets to achieve a reliable prediction depends on the considered case, i.e., geometry, materials, etc..

Fig. 5 shows LSPR characteristics (resonance wavelength and FWHM, respectively) for the nano-sinusoid chains obtained from FDTD modeling, and compares ANN outputs for a given test input data. As can be seen, there is an ideal match between the two output data sets for the same input data, including the physical dimensions of the NPs.

Figure 5(a) demonstrates how close the wavelength of ANN prediction is to the FDTD modeling result. FWHM gives an indication of the sharpness of the plasmon spectrum, i.e. damping mainly due to inter- and intra-band energy activation thresholds, which is strongly dependent on the shape and material of the NPs. Figure 5(b) compares the FWHM values for the nano-sinusoid NP structure. These coefficients are attained during training of the ANN by applying the input/output data sets to the network.

Therefore, the trained ANN can accurately predict the plasmon spectra of the nano-structures from a set of input parameters, i.e. the physical dimensions of the nano-particles, which completely matches with the FDTD modeling results.

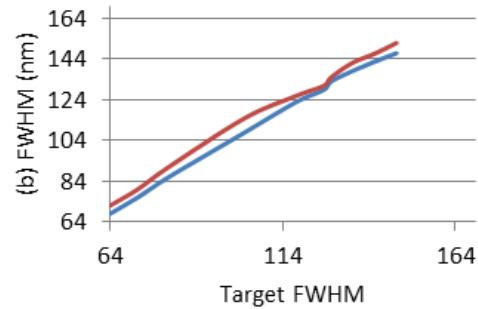
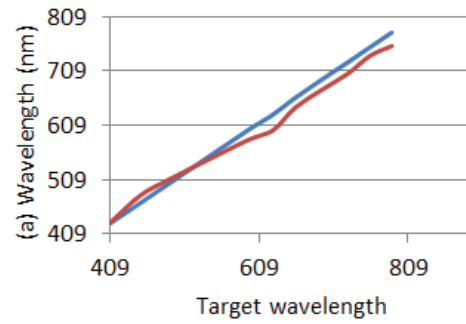


Figure 5. Comparison of (a) resonance wavelength and (b) FWHM attained from FDTD modelling (red colour) and ANN modelling (blue colour) versus target values for nano-sinusoid NPs.

4. CONCLUSION

In this paper, the interaction of nano-sinusoid NPs in terms of the LSPR phenomenon was statistically investigated. The multilayer perceptron ANN employed to model the most important features of the LSPR spectrum, i.e. resonance wavelength and FWHM, as functions of the physical dimensions of the NPs structure. These ANNs can be utilized to predict the characteristics of a LSPR spectrum of a particular NP shape before fabrication, and allows a strong reduction of the fabrication/testing phase of the development.. The results of a trained ANN applied to the test input data set ideally matches with those of the FDTD simulation.

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