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Optical Properties of Silicon-Germanium Alloy and Cuprous Oxide with Their Applications in Plasmonics

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***Abstract*—The single-pole Lorentz model parameters for Silicon-Germanium Alloy (1.5:1) and Cuprous Oxide are presented. An algorithm has been developed to optimize the parameters applicable to a broad frequency range. The obtained parameters have been used to determine the complex relative permittivity for these two materials. To verify the obtained results, they have been compared with experimental values and a very good agreement is achieved. The associated root-mean-square (RMS) deviations are observed to be 0.15 and 0.08 respectively. Finally a plasmonic waveguide based on Metal-Dielectric-Metal (MDM) configuration constructed with silver (metal) and Cuprous Oxide (dielectric) has been analyzed and presented.**

***Keywords*— Single-pole Lorentz Model, finite-difference time-domain, surface plasmon polariton (SPP), plasmonics, metal-dielectric-metal (MDM) waveguide.**

I. Introduction

The finite-difference time-domain (FDTD) [1] is one of the most popular methods for solving electromagnetic problems. The solutions obtained using this method can cover a wide frequency range in a single run which reduces the computation time significantly. However, the modeling parameters of the materials used for simulation have to be applicable over a wide frequency range in order to get accurate results.

The original FDTD method does not account for the frequency dependent material dispersion property. A number of FDTD based algorithm have been proposed by researchers for the analysis of dispersive materials. The constitutive modeling parameters for materials need to be specified as constants in all FDTD based simulation algorithms. Usually the single-pole Lorentz model is used to account for the dispersive property of dielectric materials. Since the equation describing this model is nonlinear in nature, it is difficult to optimize the parameters such that they are applicable to the wide range of frequencies. Several works have been done in the past by different researchers on the optimization of parameters for different materials using different models. Rakic *et al.* [2] have determined the parameters for several metals using Lorentz-Drude and Brendel-Bormann models with multiple poles. Gai *et al.* [3] have presented Modified Debye Model parameters for five metals. M. Alsunaidi *et al.* [4] obtained the parameters for aluminum gallium arsenide (AlGaAs) using single-pole Lorentz model.

In this paper, we present the single-pole Lorentz model parameters for Silicon-Germanium alloy (1.5:1) and Cuprous Oxide. The parameters have been optimized using an algorithm based on nonlinear least square method. We determine the complex relative permittivity using the obtained parameters and compare the results with experimental values [5]. The RMS deviations are found to be only 0.15 and 0.08 respectively. At the end, we present an analysis of Surface Plasmon Polariton propagation through a Metal-Dielectric-Metal waveguide constructed with Cuprous Oxide. To the best of our knowledge, this is for the first time one optimizes the model parameters for these materials applicable for wide frequency range. This study is important because it enables the researchers to model the frequency dependent dispersive property of materials which is necessary to achieve better accuracy in the simulation results.

II. Material Model and Optimization Method

A. *Material Model*

The frequency dependent complex permittivity function for single-pole Lorentz model is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\omega_o^{\,2}(\varepsilon_s - \varepsilon_\infty)}{\omega_o^{\,2} + j2\delta\omega - \omega^2} \qquad (1)$$

where, ε_∞ is the infinite frequency relative permittivity, ε_S is the zero frequency relative permittivity, *j* is the imaginary unit, δ is the damping co-efficient and ω_o is the frequency of the pole pair.

From (1), it can be observed that single-pole Lorentz model can be described by four parameters which are ε_∞, ε_S, δ and ω_o. These four parameters are independent and need to be optimized. The next step is to develop a nonlinear method to optimize these parameters since the equation describing the model is itself nonlinear.

B. *Optimization Method and Results*

The method we adopt for the solution of the nonlinear equation is the subspace Trust-Region method [6]. The advantage of this method is that it can handle the situation when Jacobian matrix is singular. We utilized the optimization toolbox of MATLAB in order to optimize the parameters for the materials. The program we developed is based on least-squares method and the core of the program is a large-scale algorithm [7].

TABLE I. OPTIMIZED PARAMETERS FOR SILICON-GERMANIUM ALLOY AND CUPROUS OXIDE FOR SINGLE POLE LORENTZ MODEL

Parameters	Silicon-Germanium Alloy	Cuprous Oxide
ε_∞	1.21×10^2	1.41×10^2
ε_S	3.59×10^2	2.49×10^2
δ	7.1×10^{10}	6.1×10^{10}
ω_o	5.3×10^{15}	0.53×10^{16}
Range of Wavelength (nm)	900-1300	800-1500
RMS Deviation	0.15	0.08

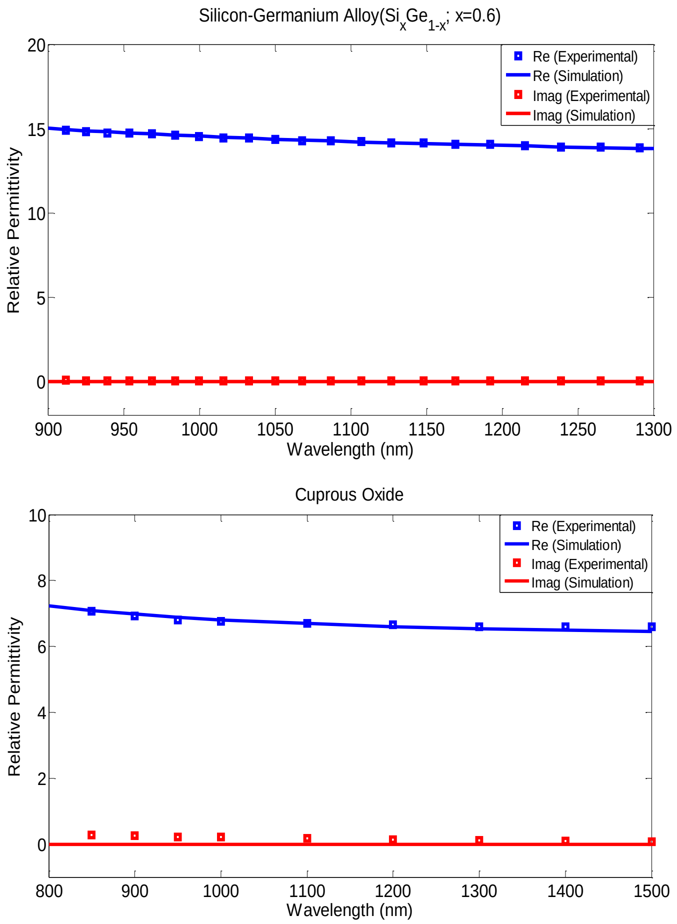


Figure 1. Comparison of relative permittivity between our results and experimental values [5]. Here blue color indicates real part and red color indicates imaginary part of the complex relative permittivity.

We need to define the initial values and the program finds the optimal values in order to minimize $f(\varepsilon_\infty, \varepsilon_s, \delta, \omega_o)$.

$$\min f(\varepsilon_\infty, \varepsilon_s, \delta, \omega_o) = \frac{1}{2}\sum_j \| \hat{\varepsilon}_j(\varepsilon_\infty, \varepsilon_s, \delta, \omega_o) - (\varepsilon_j^{'} - i\varepsilon_j^{''}) \|_2^2 \quad (2)$$

However, there are some necessary conditions that should be fulfilled in order to make this method to work. The object function should be continuous and the number of equations should be as many as the number of parameters to be optimized.

III. Application In Plasmonic Waveguide

In this section, we provide an example of SPP propagation in a plasmonic waveguide based on MDM configuration using the optimized Cuprous Oxide parameters. We also simulated the MDM waveguide using AlGaAs as the dielectric material and determined the SPP propagation length along the waveguide for both these cases. The simulation presented here is based on the Finite-Difference Time-Domain (FDTD) method proposed by Yee [1]. A general ADE-FDTD algorithm [8] is used to incorporate the frequency-dependent permittivity terms in the simulation process.

The six-pole Lorentz-Drude model is used to model silver and single-pole Lorentz model is used to model Cuprous Oxide.

The required parameters for simulation for different materials have been obtained from different resources. For silver (metal) we have used the parameter values obtained by Rakic *et al.* [2] and for AlGaAs we have taken the values determined by M. Alsunaidi *et al.* [4].

We take the step size as $\Delta x = 5\,\text{nm}$, $\Delta y = 5\,\text{nm}$ and the time step as $\Delta t = \dfrac{0.95}{c\sqrt{\dfrac{1}{\Delta x^2} + \dfrac{1}{\Delta y^2}})}$, where c is the speed of light and taken as $c = 3\times10^8\,ms^{-1}$.

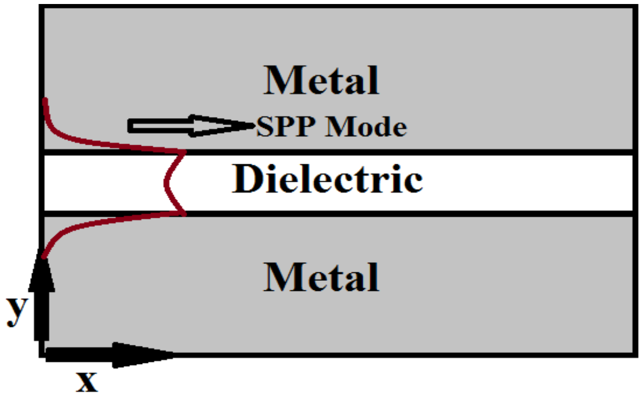


Figure 2. Schematic diagram of the MDM waveguide structure used for simulation.

In order to ensure the stability with minimum numerical dispersion we set the mesh parameters of the FDTD algorithm accordingly. The Perfectly Matched Layer (PML) [9] is integrated into the simulator in order to prevent back reflections from the boundaries.

The schematic diagram of the plasmonic waveguide we simulated is given in figure 2. The width of the dielectric layer is taken as 70nm and for metal it is taken as 465nm.

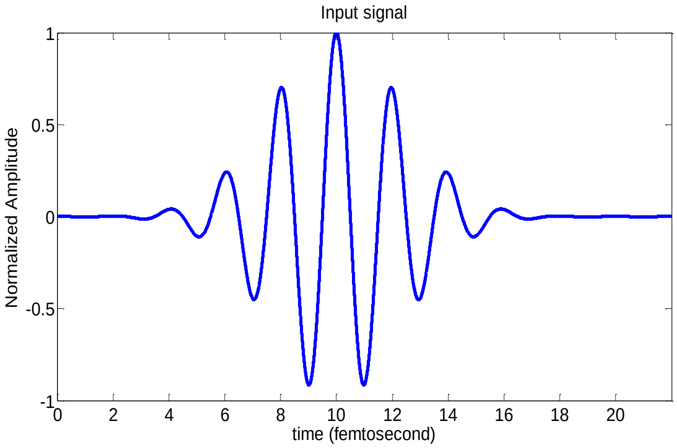


Figure 3. The normalized input signal in time domain.

At first, we run the simulation using the input signal given above in order to generate the SPP mode which is given in figure 4. Then we pumped the SPP mode into the waveguide modulated by a Gaussian pulse having a characteristic pulse width of 3 femtoseconds. The wavelength of the carrier signal is taken as 1200nm.

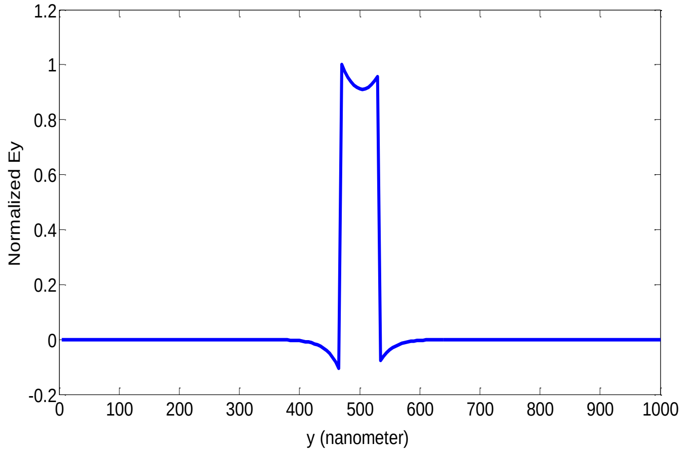
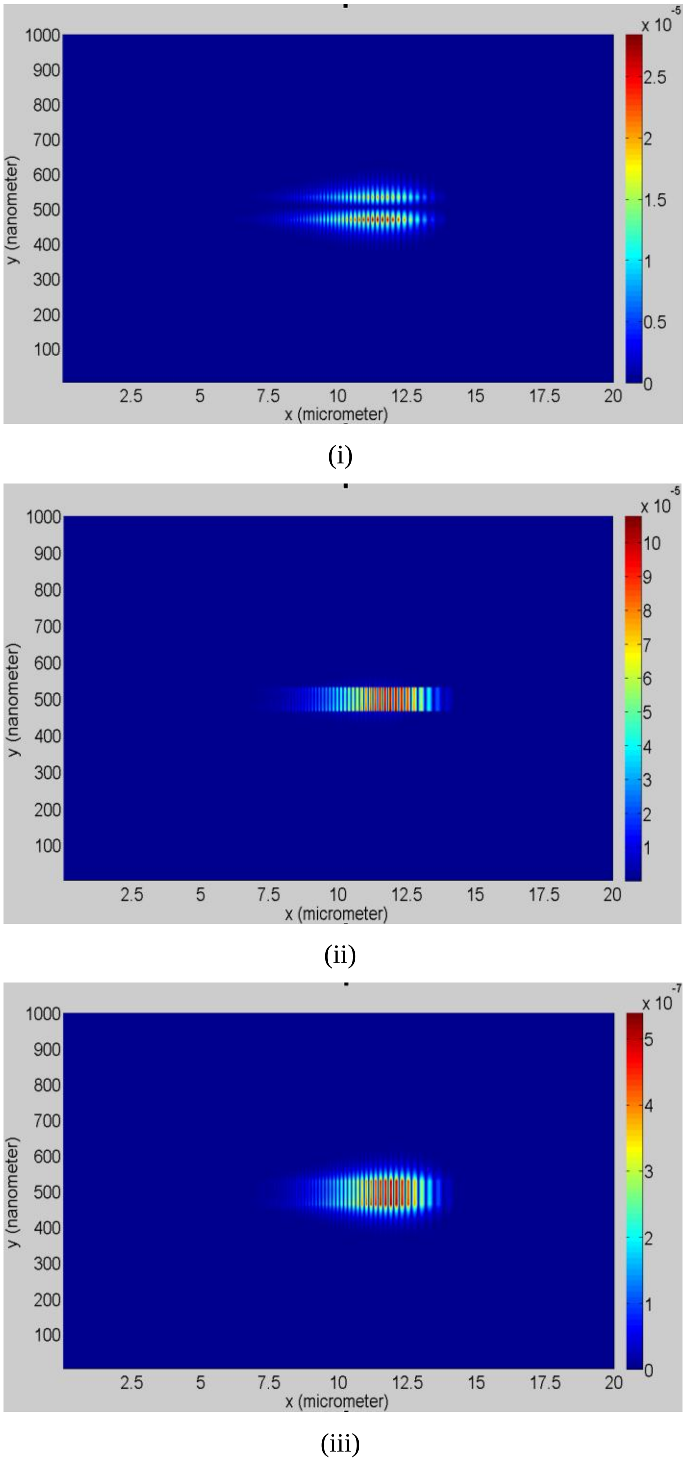


Figure 4. Normalized Ey profile pumped into the waveguide.

The Ex, Ey and Hz field distributions are given in figure 5(i) to figure 5(iii). We determine the propagation length of the SPP along the MDM waveguide constructed with Cuprous Oxide for the carrier signal wavelength of 1200nm which is given in fig. 6. The propagation length of SPP in an MDM waveguide made with AlGaAs is also presented. In case of both waveguides we keep the input signal and width of materials same. From figure 6 we can see that the propagation length for the waveguide made with Cuprous Oxide is more than 10μm while for the waveguide made with AlGaAs, it is about 7.5μm. This indicates that SPP loses power at a lesser rate in the case of the waveguide constructed with Cuprous Oxide. Therefore, Cuprous Oxide can be used to support long-range propagation of SPP.



(i)

(ii)

(iii)

Figure 5. (i) Ex (ii) Ey and (iii) Hz field distribution of the simulated MDM waveguide using Cuprous Oxide.

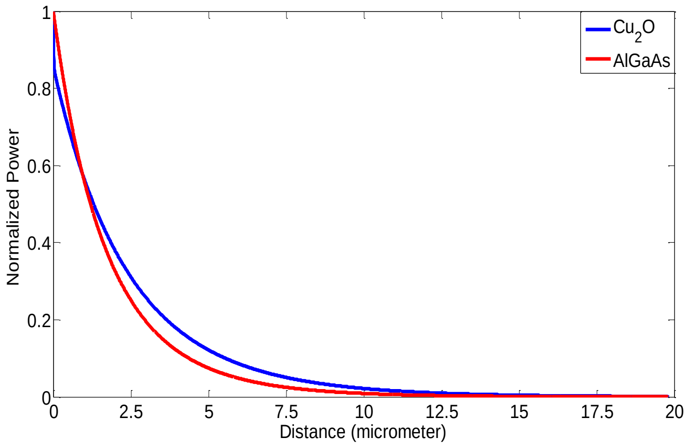


Figure 6. The normalized power profile for carrier signal wavelength of 1200nm.

IV. Conclusion

We optimized the single-pole Lorentz model parameters for Silicon-Germanium alloy and Cuprous Oxide using nonlinear least-squares algorithm. The validation of the optimized parameters has been done by comparing the obtained results with experimental results [5]. At the end, we present an application of the optimized parameters in an MDM waveguide. We determine the propagation length of the waveguide using cuprous oxide and find out that it shows promising results in terms of efficiency. We expect that this analysis will be useful for the fabrication of integrated photonic devices and other optical research works.

Acknowledgment

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