Extraction of optimized parameters for $Si_{0.6}Ge_{0.4}$ material and SPP mode propagation through $Si_{0.6}Ge_{0.4}$/Ag/$Si_{0.6}Ge_{0.4}$ waveguide

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The Lorentz model and modified Debye model (MDM) parameters for $Si_{0.6}Ge_{0.4}$ are presented. A nonlinear optimization algorithm is developed. The obtained parameters are used to determine the complex relative permittivity of $Si_{0.6}Ge_{0.4}$, and compared with the experimental data for validation. Finally the obtained parameters are used to analyze the properties of symmetric surface plasmon polariton (SPP) mode propagation in a dielectric-metal-dielectric (DMD) material constructed with silver (Ag) and $Si_{0.6}Ge_{0.4}$ for further verifying the extracted parameters.

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Plasmonics has attracted a lot of research interest due to its ability to overcome the diffraction limit[1-3]. The incredible property of surface plasmon polariton (SPP) indicates its potential applications in biosensing[4], Bragg reflectors[5], sub-wavelength imaging[6,7], metamaterials[8] and enhanced light absorption in solar cells[9,10].

Plasmonic devices available at present face substantial challenge because of the losses encountered in the constituent materials. These losses restrict the practical applications of the materials significantly. A lot of relative researches are going on in order to find out new plasmonic materials that can support enhanced propagation of the SPP and provide better confinement for the SPP mode. P. R. West et al[11] reported a detailed analysis on different plasmonic materials with motivation for choice of materials and important aspects of fabrication. W. Guo et al[12] presented an analysis of symmetric SPP mode propagation in Ag/Al_2O_3/Ag waveguide. Herein, we report the extraction of optimized parameters of a new dielectric material $Si_{0.6}Ge_{0.4}$ for Lorentz model and modified Debye model (MDM), and provide a detailed analysis of SPP mode propagation through $Si_{0.6}Ge_{0.4}$/Ag/$Si_{0.6}Ge_{0.4}$ waveguide. We have developed a two-dimensional simulation model based on finite-difference time-domain (FDTD) algorithm[13]. The parameters for both the models have been used separately to simulate the SPP mode propagation through the waveguide. We have also determined the same SPP mode propagation properties using analytical equations. The obtained results using both the methods have been compared and an excellent agreement can be found.

The frequency dependent permittivity function of the single-pole Lorentz model is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\omega_0^2(\varepsilon_s - \varepsilon_\infty)}{\omega_0^2 + j2\delta\omega - \omega^2}, \quad (1)$$

where ε_r is the complex relative permittivity, ε_∞ is the infinite frequency relative permittivity, ε_s is the zero frequency relative permittivity, j is the imaginary unit, δ is the damping coefficient, and ω_0 is the frequency of the pole pair. It can be observed from Eq.(1) that single-pole Lorentz model can be described by four parameters of ε_∞, ε_s, δ and ω_0. These four parameters are independent and need to be optimized if we want to model any material using Lorentz model.

The frequency dependent permittivity function of MDM is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau}, \quad (2)$$

where τ is the relaxation time. We can see from Eq.(2) that the MDM for dielectric material can be described by three parameters of ε_∞, ε_s and τ. These three parameters need to be optimized in order to model any dielectric material using MDM.

The used optimization algorithm is as follows. First we obtain the experimental values from the book of E. D. Palik[14] and use them to determine the complex relative permittivity for each material. Then the program varies the parameters which need to be optimized, and different combinations are tried to determine the complex relative permittivity. The square of the complex relative permittivity obtained using the optimized parameters is subtracted from the square of the complex relative permittivity obtained using experimental values. The squared differential term is then compared with a predetermined

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tolerance value which is close to zero, and the iteration goes on until the preset value. The flow chart is shown in Fig.1.

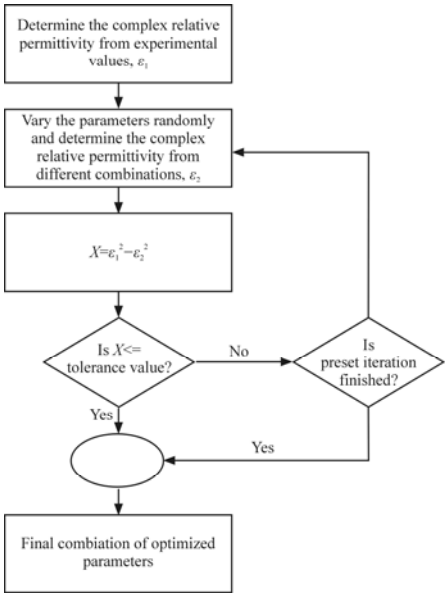


Fig.1 Flow chart of the algorithm used for parameter extraction

The variation of the modeling parameters is random. However, boundary limits are set so that the extracted parameters can meet the requirement of the FDTD method. Varying the modeling parameters in a random function is the most challenging part of the algorithm. If a linear method is used to vary the parameters, the computation time will be much higher. Since the variation is random, it takes less time to find a combination of values which produces the least squared difference. The boundary conditions which need to be maintained for the MDM parameters and to be integrated in the FDTD algorithm are $\varepsilon_\infty>1$ and $\varepsilon_s<\varepsilon_\infty$.

This algorithm is applicable for the single-pole model only. The obtained results will be inaccurate if it is used for parameter extraction of multiple-pole models.

A two-dimensional simulation model has been developed based on FDTD[13] algorithm in order to simulate the $Si_{0.6}Ge_{0.4}$/Ag/$Si_{0.6}Ge_{0.4}$ waveguide. The original FDTD algorithm formulated by Yee doesn't account for the frequency dependent permittivity of the materials. Therefore, we have used the auxiliary differential equation (ADE)-general FDTD algorithm in order to incorporate the frequency dependent dispersion property of the materials. This algorithm can handle the case when there are materials with different dispersion properties. The perfectly matched layer[15] is also used in order to avoid the reflection of incident wave from the boundaries. The $Si_{0.6}Ge_{0.4}$ /Ag/ $Si_{0.6}Ge_{0.4}$ waveguide is used for simulation. The widths of the Ag layer and $Si_{0.6}Ge_{0.4}$ layer are taken as 60 nm and 500 nm, respectively. The schematic diagram of the dielectric-metal-dielectric (DMD) waveguide for numerical analysis is given in Fig.2.

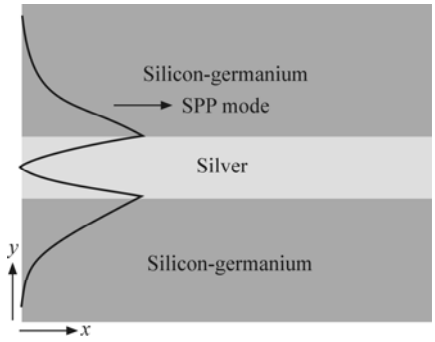


Fig.2 Schematic diagaram of the DMD waveguide used for the numerical analysis

The step size is taken as Δx=2 nm, Δy=2 nm, and the time step is set as $\Delta t = 0.95\Big/ c\sqrt{\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}}$, where c is the speed of light in vacuum and taken as $c=3\times10^8$ m/s. We find that it is sufficient to satisfy Courant stability condition[16].

The optimized modeling parameters for both Lorentz model and MDM using our developed algorithm are presented in Tab.1. It can be observed from Tab.1 that a root mean square (RMS) deviation for Lorentz model is 0.15, and that for MDM is 0.3710, which both indicate the robustness and accuracy of our optimization algorithm.

Tab.1 Optimized parameters of $Si_{0.6}Ge_{0.4}$ for single-pole Lorentz model and MDM

Parameter	Single-pole Lorentz model	MDM
ε_∞	$(1.21)^2$	14.2996
ε_s	$(3.59)^2$	1.519
δ (rad/s)	7.1×10^{10}	N/A
ω_0 (rad/s)	5.3×10^{15}	N/A
τ (s)	N/A	2.261
Wavelength range (nm)	900–1300	900–1300
RMS deviation	0.15	0.3710

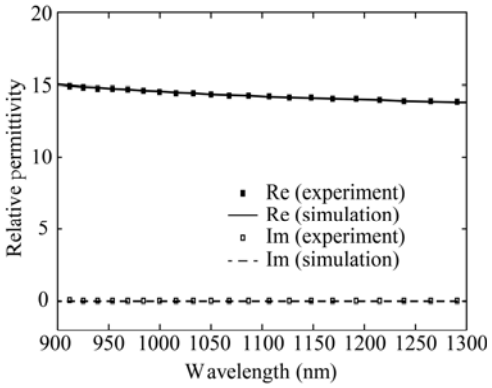
The complex relative permittivity for $Si_{0.6}Ge_{0.4}$ has been determined by using both the extracted parameters and the experimental values[14]. Then the real and imaginary parts separated from the complex relative permittivity are presented in Fig.3. It is clearly seen from Fig.3 that the real and imaginary parts of the complex relative permittivity obtained using extracted parameters agree very well with those obtained from the experimental values for both models[14].

The SPP wavelength is given by

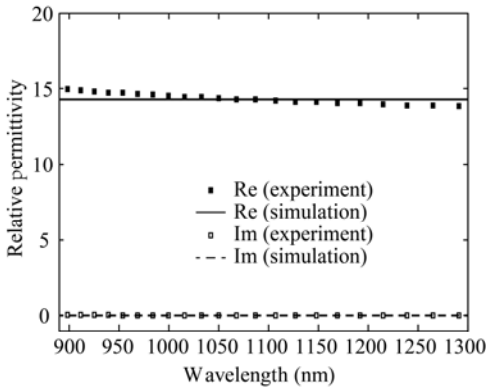
$$\lambda_{SPP} = \lambda_0\sqrt{\frac{\varepsilon_d+\varepsilon_m'}{\varepsilon_d\varepsilon_m'}}, \tag{3}$$

where λ_0 is the free space wavelength, ε_d is the real part of the complex relative permittivity of dielectric and ε_m' is the real part of the complex relative permittivity of metal.

We calculate the SPP wavelength using both equation and simulation. The obtained results are then compared, and a very good agreement is found between the analytical and numerical results, which can be observed in Fig.4.



(a) Lorentz model



(b) MDM

Fig.3 Real and imaginary parts of the complex relative permittivity for $Si_{0.6}Ge_{0.4}$ obtained using extracted parameters and experimental values for single-pole Lorentz model and MDM

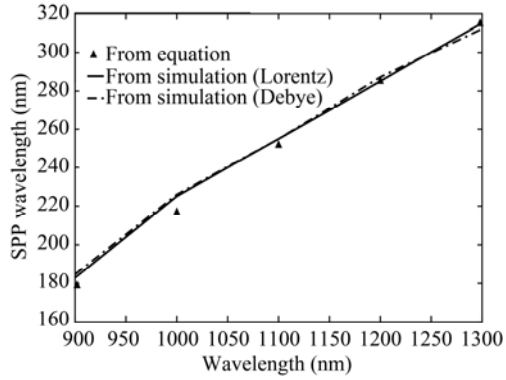


Fig.4 SPP wavelength calculated analytically and numerically

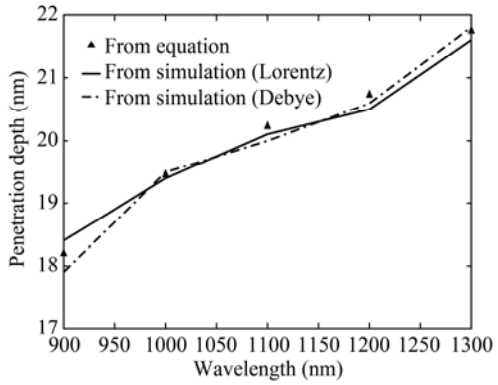
The next property is the field penetration depth into Ag and $Si_{0.6}Ge_{0.4}$ layers. The penetration depths into dielectric and metal are given by

$$\delta_{\mathrm{d}} = 1/k_{\mathrm{o}} \left| (\varepsilon_{\mathrm{d}} + \varepsilon_{\mathrm{m}}^{'}) / \varepsilon_{\mathrm{d}}^{2} \right|^{0.5}, \tag{4}$$

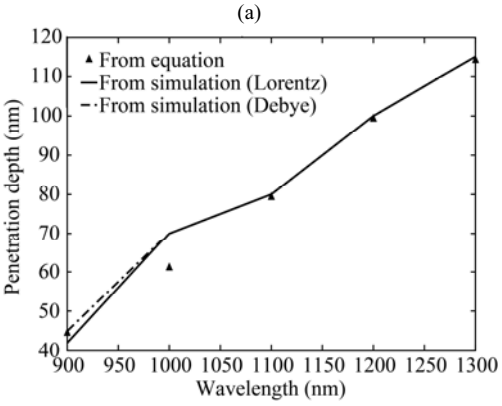
$$\delta_{\mathrm{m}} = 1/k_{\mathrm{o}} \left| (\varepsilon_{\mathrm{d}} + \varepsilon_{\mathrm{m}}^{'}) / \varepsilon_{\mathrm{m}}^{2} \right|^{0.5}, \tag{5}$$

where $k_0=2\pi/\lambda_0$ is the wave-vector for light in free space.

The field penetration depths into Ag and $Si_{0.6}Ge_{0.4}$ layers are determined by using the equations for different input signal wavelengths and the simulation for both single-pole Lorentz model and MDM. An excellent agreement is found between the results obtained using the two techniques which are presented in Fig.5. Therefore, it is evident that our extracted parameters for $Si_{0.6}Ge_{0.4}$ for the two models are valid.



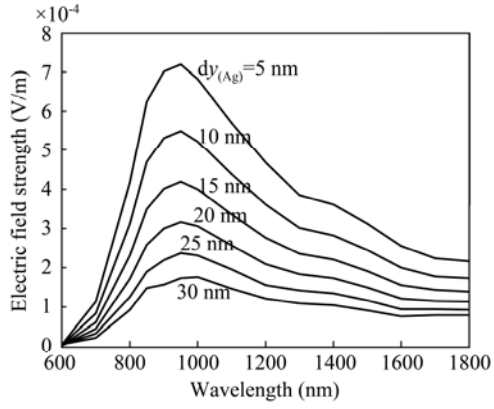
(a)



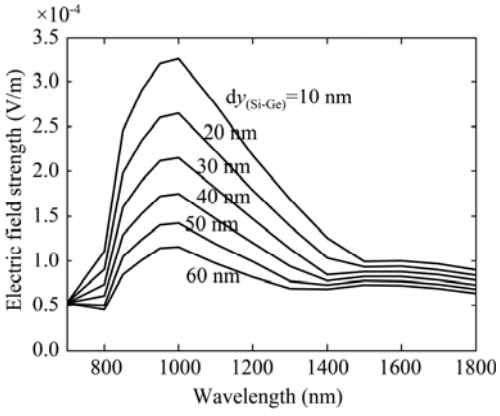
(b)

Fig.5 Field penetration depths into (a) Ag layer and (b) $Si_{0.6}Ge_{0.4}$ layer calculated analytically and numerically

The electric field strengths at different distances from the top surface of Ag/$Si_{0.6}Ge_{0.4}$ are given in Fig.6 for single-pole Lorentz model and in Fig.7 for MDM.

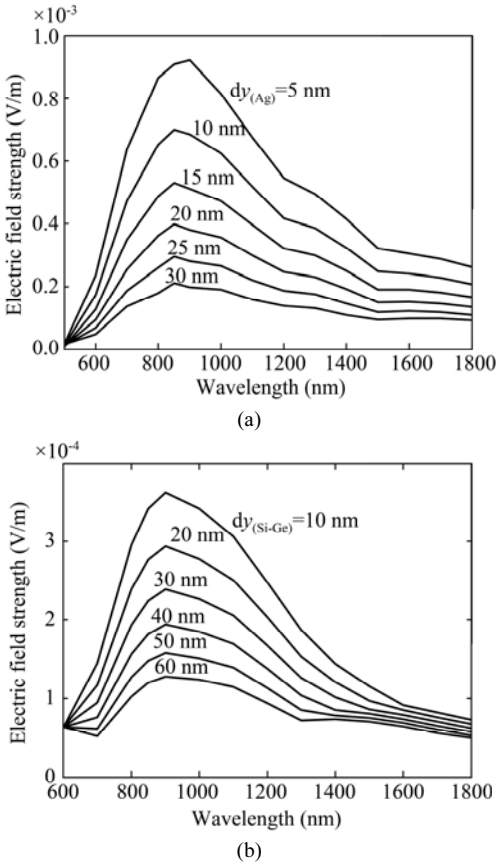


(a)



(b)

Fig.6 Electric field strength as a function of distance for single-pole Lorentz model in (a) Ag layer and (b) $Si_{0.6}Ge_{0.4}$ layer



(a)

(b)

Fig.7 Electric field strength as a function of distance for MDM in (a) Ag layer and (b) $Si_{0.6}Ge_{0.4}$ layer

It can be observed from Figs.6 and 7 that the electric field strength decreases when we go further from the top surface of Ag/ $Si_{0.6}Ge_{0.4}$ into both Ag and $Si_{0.6}Ge_{0.4}$ layers. It happens due to the skin effect of the symmetric SPP mode in both Ag and $Si_{0.6}Ge_{0.4}$ layers. The resonance mode is also observed in Figs.6 and 7.

We report the optimized parameters of $Si_{0.6}Ge_{0.4}$ for single-pole Lorentz model and MDM. The optimized parameters are validated by being compared with the experimental results. We present an analysis on SPP mode propagation through the $Si_{0.6}Ge_{0.4}$/Ag/$Si_{0.6}Ge_{0.4}$ waveguide. In each case, the numerical result agrees well with the analytical result, which further validates the extracted parameters. We expect that this study will provide better understanding about light-matter interaction at the nanometer-scale and supply new ways of manipulating light in the integrated photonic devices, leading to applications in optical communications.

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