Optical Semiconductor Surface-Plasmon Dispersion Including Losses Using the Drude-Lorentz Model

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Abstract — **Theoretical solutions are obtained for the propagation of electromagnetic waves at optical frequencies along a semiconductor/dielectric interface when losses are taken into account in the form of a complex dielectric function. A combination method for the dielectric function, comprised of the best features of the Drude and Lorentz models, is herein proposed. By including the loss term in both models, we were able to obtain numerical solutions for the plasma dispersion curve of the semiconductor/dielectric interface. The surface plasmon waves, when excited, become short wavelength waves in the optical frequency or THz region. A silicon/air structure was used as our semiconductor/dielectric material combination, and comparisons were made to optical plasmons generated without losses. Our initial numerical calculation results show enormous potential for use in several applications.**

Index Terms—**Semiconductor optical plasmons, surface plasmon polaritons, optical plasmon, Drude-Lorentz model, plasma dispersion.**

I. INTRODUCTION

THE fundamental optical excitation that is confined to a metal/dielectric interface is the Surface Plasmon Polariton (SPP), as described by Ritchie [1]. The term SPP comes from coupled modes, which can be used to confine light and increase the electromagnetic fields at an interface between two media, of which at least one is conducting [2-5]. Plasmonics in a semiconductor are taking an increasingly prominent role in the design of future silicon-based optoelectronic chips [6].

Optical plasmons have been shown to have many applications [2, 3] and are generally excited using metal/dielectric interfaces due to the high concentration of charge carriers in metals. SPPs in semiconductor/dielectric interfaces have recently received considerable interest, and the use of a semiconductor/dielectric interface to support optical plasmons has been numerically shown in [7], albeit without the inclusion of losses. We therefore wish to take this a step further by including the loss contribution in the SPP dispersion relation. The loss is introduced through the complex dielectric function of the semiconductor. Little attention has thus far been paid to this phenomenon because it is generally very difficult to deal with. The SPPs dispersion and the resonance frequency depend on the interface configuration [2, 7].

Unlike metals, the semiconductor permittivity theory can be extremely complex, since it depends on the doping concentration of the semiconductor, which also determines the number of bound and free charge carriers in the material. In a semiconductor, plasma frequency can be determined by the effective carrier mass as well as the doping concentration. Two of the more difficult tasks are to confine light and increase the electromagnetic fields near the interfaces. The losses are related to the plasma dispersion; however, they affect the shape of the plasmon dispersion curve near the plasma frequency.

Our goal is to develop a theoretical treatment to find a suitable model for the dielectric function of semiconductors. Starting with the Drude model, which is commonly used to describe the dielectric function of metals, we seek to modify and adapt it for semiconductors by adding the Lorentz model.

We proceed by solving Maxwell's equation for the interface between the dielectric and the semiconductor, and using the dielectric function described by the Drude-Lorentz model to obtain the dispersion relation.

This paper is organized as follows: A brief theory and background of models describing dielectric permittivity is addressed in Section II. In Section III, numerical results are presented and discussed, and Section IV summarizes the results and conclusions.

II. THEORETICAL ANALYSIS

In this section, we discuss different models, one of which is selected for our approach. The Drude model, Lorentz model, and a combination of both models (i.e., Drude-Lorentz model) are presented and discussed. Starting with a semiconductor/dielectric interface, we seek to obtain a surface plasmon wave traveling along that interface (z-axis) in the form [7]:

$$E_{x,y} = E_{x,y}^{d,s}\delta_{d,s} \quad (1)$$

$$\delta_{d,s} = e^{-i\omega t}e^{i\gamma_{d,s}}e^{i\beta z} \quad (2)$$

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where ω is the angular frequency, and $\gamma_{d,s}$ and β are the transverse and longitudinal propagation constants, respectively.

This assumed form of an evanescent wave is substituted in the Maxwell's equations:

$$\nabla \times H = J_q + \varepsilon_o \frac{\partial E}{\partial t} + \frac{\partial P}{\partial t} \qquad (3)$$

$$\nabla \times E = -\mu_o \frac{\partial H}{\partial t} \qquad (4)$$

$$\nabla . H = 0 \qquad (5)$$

$$\nabla . \left(\varepsilon_o \frac{\partial E}{\partial t} + \frac{\partial P}{\partial t}\right) = \frac{\partial \rho}{\partial t} \qquad (6)$$

$$D = \epsilon E \qquad (7)$$

$$J = \sigma E \qquad (8)$$

To complete the development of optical plasmon in semiconductors theoretically, the notation of damping has to be described. From a basic perspective, the result of the surface plasmon dispersion equation becomes complex when losses are accounted for. This is directly related to the complex dielectric constant; in order to characterize the dispersion, damping, and excitation of the plasmon, its imaginary part needs to be included. Then the dielectric permittivity equation becomes complex. The dielectric constant is one of the most important factors to assess for future technology applications [6].

Applying the appropriate boundary conditions on both sides of the interface yields the dispersion equation below as:

$$(\varepsilon_S^2 - \varepsilon_D^2)\left[\frac{k^2 \varepsilon_S \varepsilon_D - \beta^2 \varepsilon_S - \beta^2 \epsilon_D}{\varepsilon_S \varepsilon_D (\varepsilon_S + \varepsilon_D)}\right] = 0 \qquad (9)$$

where,

$$k = \frac{\omega}{c} \qquad (10)$$

ε_S is the dielectric permittivity of the semiconductor, ε_D is the dielectric permittivity of the dielectric, c is the speed of light, and k is the wavenumber.

To be able to account for losses, we used a complex dielectric constant in the form:

$$\varepsilon_r = \varepsilon' + j\varepsilon'', \qquad (11)$$

where, ε_r is the relative permittivity, ε' is a real part, and ε'' is the imaginary part. ε_r can be represented by different models, so before presenting our proposed Drude-Lorentz model, we present the Drude model, which is commonly used for metals and highly doped semiconductors.

A. Drude Model

This model was proposed by Paul Drude in 1900 to explain the transport properties of electrons in metals [8, 17] and has also been adapted for semiconductors [9, 10]. The Drude dielectric function is given by

$$\varepsilon_r = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + j\gamma)} \qquad (12)$$

where ε_∞ is the high frequency permittivity and ω_p is the plasma angular frequency given by [11]

$$\omega_p = \sqrt{\frac{ne^2}{\varepsilon_o m^*}} \qquad (13)$$

m, e, and n are the electron effective mass, the electron charge, and the carrier density, respectively. γ is the damping term, and ε_o is the permittivity of free space.

The Drude model is the simplest classical treatment of optical properties of metals. It considers the valence electrons of the atoms to be free. In addition, it is used for semiconductors when free carrier density introduced through doping is sufficiently high to cause the semiconductor behave similarly to a simple metal. However, in reality, this model has limitations. For example, it does not account for spatial dispersion, which exists when the dielectric constant depends on the wave-vector. Moreover, it does not account for the bound electrons and holes in semiconductors.

B. Lorentz Model

The Lorentz model can be used to describe the frequency response of many materials and typically shows strong dispersions around the resonant frequency [12, 15,18]. It is mostly suited for materials that have bound electrons, with the possibility of having many oscillators in a given system [8, 11, 13, 14]. The expression of the dielectric function for a single Lorentz oscillator is given by:

$$\varepsilon_r = \varepsilon_\infty - \frac{\Delta_\varepsilon \omega_p^2}{j\omega^2 + j\gamma\omega + \omega_o} \qquad (14)$$

where ω_o is the resonance frequency and is considered to be equal to an energy band gap of a semiconductor. Δ_ε is a weighting factor given by $\Delta_\varepsilon = \varepsilon_{st} - \varepsilon_\infty$, with ϵ_{st} being the static permittivity.

As mentioned, the Lorentz model usually shows strong dispersions around the resonant frequency [12, 14] and is valid only when the photon energy is well below the band gap of the semiconductor. Thus, it cannot be used alone to describe the permittivity of semiconductors.

To overcome this limitation, we propose the use of the Drude-Lorentz model to describe the dielectric function of semiconductors in the optical frequency range. The proposed dielectric function is given by:

$$\varepsilon_r = \varepsilon_\infty - \frac{\omega_p^2}{\omega(\omega + j\gamma)} + \frac{\Delta_\varepsilon \omega_p^2}{j\omega^2 + j\gamma\omega + \omega_o} \qquad (15)$$

This model is chosen to enable us to take advantage of semiconductors at optical frequencies and search for a possibility of an optical plasmon existence in that range.

III. DISCUSSION & RESULT

A Matlab symbolic tool has been used to implement the above models. From Equation (9), we insert the desired model of the dielectric function and proceed to calculate the dispersion relation. Before we examine the possible development of the models that work for both materials (i.e., semiconductors and metals), we need to address the question

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of why it should even be done. The basic answer is to gauge the effect of the loss of coupling plasmons, especially in semiconductors. The slight change of a dielectric permittivity and the damping values are taken into account.

We commence by discussing the details of all of the above models. To solve this dilemma, it is necessary to assume that the system is lightly damped. Based on this assumption, we can then ignore the damping term at first, and later add the loss term for comparison. Next, we recall Equations (3) to (8) and substitute them in the model equation. Doing so, and satisfying the boundary conditions for fields in both media, one can find the dispersion equation for the Drude model without loss as:

$$\begin{aligned}&-\omega^6\left(\varepsilon_s\epsilon_d^2-\varepsilon_s^2\epsilon_d\right)\\&+\omega^2\left(\beta^2c^2\varepsilon_s^2-\beta^2c^2\varepsilon_d^2+\varepsilon_d^2\omega_p^2\right.\\&\left.-2\varepsilon_s\varepsilon_d\omega_p^2\right)\\&+\omega^2\left(2\varepsilon_d\beta^2c^2\omega_p^2+\varepsilon_d\omega_p^2\right)\\&-\beta^2c^2\omega_p^2\\&=0\end{aligned}\tag{16}$$

where, ε_s is a semiconductor dielectric permittivity, ϵ_d is a dielectric permittivity, and ω_p is the plasma frequency.

Neglecting the losses in this equation and setting a classical metal/air interface as $\varepsilon_S=\varepsilon_D=1$ [7] yields the well-known plasma dispersion equation with well-known solution:

$$-\omega_p^2\omega^4-\omega^2\left(2\beta^2c^2\omega_p^2+\omega_p^4\right)+\beta^2c^2\omega_p^4=0 \tag{17}$$

Figure 1 shows the dispersion relation of surface plasmons propagating along a silicon/air boundary.

According to the generalized Drude theory, the complex dispersion equation is obtained. Equation (18) below is the resulting plasma dispersion equation obtained when losses are included in the Drude model, through the damping frequency, γ.

$$\begin{aligned}-\Big(\omega^2\left(3c^2\omega_p^4\beta^2-2c^2\omega_p^2\beta^2\gamma^2+\omega_p^6\right)&\\-\omega^4\left(2c^2\omega_p^2\beta^2+2\omega_p^4-\omega_p^2\gamma^2\right)&\\+\omega_p^2\omega^6-c^2\omega_p^6\beta^2+c^2\omega_p^2\beta^2\gamma^2\Big)&\\=0&\end{aligned}\tag{18}$$

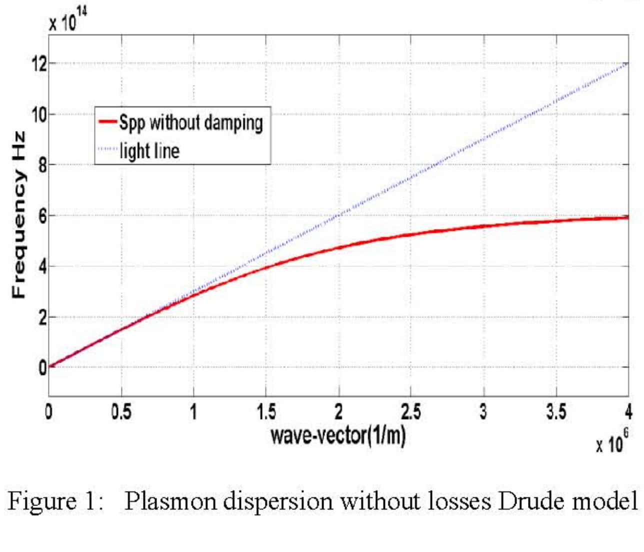

Figure 1: Plasmon dispersion without losses Drude model

As can be concluded from the dispersion relationship plotted in Figure 2, the blue straight line shows the light line $\omega=kc$. When damping is taken into account, we observe a visible drop of the surface plasmon frequency from 590 THz to about 432 THz, which gives us a surface plasmon wave in the optical frequency range.

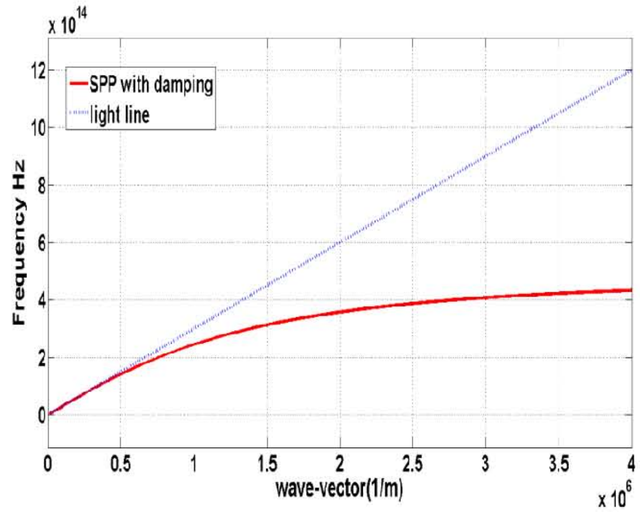

Figure 2: Plasmon dispersion with damping

Following the same steps as previously and by inserting the Drude-Lorentz model function in Equation (9) and rearranging the terms, one obtains:

$$\begin{aligned}&-(\omega^2\left(\varepsilon_s^2\omega_p^2+\beta^2c^2\Delta_\varepsilon\omega_p^2+\varepsilon_s\Delta_\varepsilon^2\omega_p^4-2\varepsilon_s\Delta_\epsilon\omega_p^4\right.\\&\left.+\varepsilon_d\omega_p^4\right)+\omega^6\left(\varepsilon_s\varepsilon_d^2-\varepsilon_s^2\varepsilon_d\right)\\&+\omega^4\left(\varepsilon_s^2\omega_p^2+\beta^2c^2\varepsilon_s^2\omega_p^2-\beta^2c^2\varepsilon_d^2-2\ \varepsilon_s\varepsilon_d\omega_p^2\right.\\&\left.-\varepsilon_s^2\Delta_\epsilon\omega_p^2+2\ \Delta_\varepsilon\varepsilon_s\varepsilon_d\omega_p^2\right)\beta^2c^2\omega_p^4+2\beta^2c^2\Delta_\varepsilon\omega_p^4\\&-\beta^2c^2\Delta_\varepsilon^2\omega_p^4)\\&=0\end{aligned}\tag{19}$$

When losses are included in the Drude-Lorentz model, the following dispersion relation is obtained:

$$\begin{aligned}&-\omega^4\left(2c^2\omega_p^2\beta^2\gamma^2+2\omega_p^4\gamma^2-\omega_p^4\gamma^2\right)\\&-\omega^2\left(3c^2\omega_p^4\beta^2\gamma^2+2\beta^2\gamma^4\omega_p^4c^2+\omega_p^6\gamma^2\right)\\&+\gamma^2\omega_p^2\omega^6-c^2\omega_p^4\beta^2\gamma^2+c^2\omega_p^6\beta^2\gamma^2\\&=0\end{aligned}\tag{20}$$

This dispersion relation of surface plasmon waves along silicon/air boundary including losses is shown in Figure 3. n-doped silicon is used in the calculations, and all physical parameters are experimental values taken from [16]. To obtain a plasma frequency in the optical range, we had to use high carrier concentrations of the order of $10^{21}/\mathrm{cm}^3$, which is feasible for silicon. By varying the plasmon frequency parameter ω_p of the semiconductor, we obtained a different curve, which has a different surface plasmon frequency, as graphed in Figure 3.

Figure 3 shows a different SPP curve than Figure 2, depicting only the real part of the Drude-Lorentz model. When $\omega_p>\gamma$ the surface plasmon frequency increases to approximately 723 THz. It should be noted that the values of

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ω_p and γ for n-doped silicon change with doping concentration.

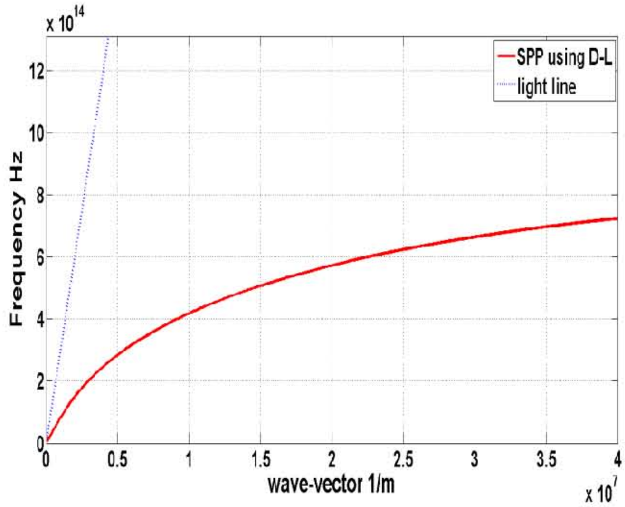

Figure 3: The Drude-Lorentz model surface plasma dispersion with damping

IV. Conclusion

Theoretical and numerical studies were conducted on plasmonic interactions at a semiconductor/dielectric interface. A brief review of the basic model theory was presented. We have shown that the inclusion of losses reduces the surface plasmon frequency. We have also proposed the Drude-Lorentz model as a model for the dielectric function of semiconductors, due to its ability to describe both free electron and bound systems simultaneously. The numerical results of the plasmon dispersion for a silicon/air interface were presented using the proposed model and were compared to the Drude model. The main contribution of this work is the derivation of a generalized dispersion relation for semiconductors, with help of the Drude-Lorentz model.

References

[1] R. H. Ritchie, Plasma Losses by Fast Electrons in Thin Films, Phys. Rev. 1957, pp.106, 874.

[2] H. Raether, *Surface Plasmons on smooth and rough surfaces and on grattings,* Springer-Verlag: Berlin, 1988, pp. 15-22.

[3] S.Maier, *Plasmonics Fundamentals and Applications*, Springer Science and business Media LLC, 1st. 2007, pp. 21-39.

[4] L. Novotny and B. Hecht, *Principles of Nano-Optics*, Cambridge, 2nd. 2008, pp. 378-414.

[5] A. V. Zayatsa, I. I. Smolyaninovb, and A. A. Maradudinc, "Nano-optics of surface plasmon polaritons," Phys. Rep. 408, 2005,pp.131–314.

[6] B. Yao, Z. B. Fang, Y. Y. Zhu, T. Ji, and G. He "A model for the frequency dispersion of the high-k metal-oxidesemiconductor capacitance in accumulation" Applied Physics Letters 100, 2012, pp. 222903/1-3.

[7] Michael Cada and Jaromír Pištora "Optical Plasmons in Semiconductors" ISMOT conference, June 20-23, 2011.

[8] Mark Fox, *Optical Properties of Solids*, 2ed, Oxford University Press, 2010, pp. 33-44.

[9] M. Kuttge, H. Kurz, J. G. Rivas, J. A. Sánchez-Gil, and P. H. Bolívar, "Analysis of the propagation of terahertz surface plasmon polaritons on semiconductor groove gratings," J. Appl. Phys., vol. 101, no. 2, 2007, pp. 023707-1–023707-6

[10] Paul R. West, Satoshi Ishii, Gururaj V. Naik, Naresh K. Emani, Vladimir M. Shalaev, and Alexandra Boltasseva, "Searching for better plasmonic materials", Laser Photonics Rev. 4, No. 6, 2010., pp. 795–808

[11] K. H. Lee, I. Ahmed, R. S. M. Goh, E. H. Khoo, E. P. Li, and T. G. G. Hung, "Implementation of the FDTD method based on the Lorentz-Drude model on GPU for plasmonics applications", Progress In Electromagnetics Research, Vol. 116, 2011, 441- 456,.

[12] J. G. Rivas, J. A. Snchez-Gil, M. Kuttge, P. H. Bolivar, and H. Kurz, "Optically switchable mirrors for surface plasmon polaritons propagating on semiconductor surfaces," Phys. Rev. B, vol. 74, 2006, pp. 245-324,.

[13] C. Janke, J. G. Rivas, P. H. Bolivar, and H. Kurz, "All optical switching of electromagnetic radiation through subwavelength apertures," Opt. Lett.,vol. 30, no. 18, 2005, pp. 2357-2359,.

[14] I. Ahmed, E. Khoo, O. Kurniawan, and E. Li, Modeling and simulation of active plasmonics with the FDTD method by using solid state and Lorentz–Drude dispersive model, J. Opt. Soc. Am. B / Vol. 28, No. 3, 2011, pp. 325-359.

[15] I. Ahmed,E. Khoo,O. Kurniawan,and E. Li, Modeling and simulation of active plasmonicswith the FDTD method by using solid state and Lorentz–Drude dispersive model, J. Opt. Soc. Am. B / Vol. 28, No. 3, 2011, pp. 325-359.

[16] Y. Laghla, E. Scheid, Optical Study of Undoped, B or P-doped polysilicon, Elsever, Thin Solid Film 306, 1997, pp. 67-73.

[17] S.Chuang, *Physics of Photonic Devices*, 2ed. Wiley,2009,pp.193-196.

[18] Aaron Hryciw, Young chul Jun and mark l. Brongersma, "Plasmonic: Electrifying plasmonics on silicon: Nature Materials 9, 2010, pp.3-4