Simulation of Copper Thin Film Thickness Optimization for Surface Plasmon using the Finite Element Method

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Abstract: This paper presents a computer simulation of optical activations based on the Kretschmann configuration using a prism for the observation of the surface plasmon wave. This is according to the condition of the dispersion relation. The analysis of the electric field of the surface plasmon wave which appears at the interface between the metal layer and the air layer is done by using the Finite Element Method (FEM). The simulation is performed using the COMSOL Multiphysics software which supports the FEM. The objective of our experiment is to find the most suitable thickness of the metal thin film which is most suitable for the surface plasmon excitation when activated by 632.5 nm red laser light source. The red laser light source is commonly available and also very economical. The metal used in our work is copper which is an economical noble metal and gives better conductivity than gold. The findings from the simulation will be used in the future high precision physical experiments. The outcome of this research project, the surface plasmon wave on copper thin film, is expected to be used in bio-molecular detectors or high speed THz communications.

1 INTRODUCTION

During the past decades, the need to verify and process data by using optics have been growing and developing rapidly. Optical sensors which are able to detect bio-molecular objects such as DNA protein are widely available. They have both sensitivity and size advantages over non-optical sensors (Anker et al., 2008). These optical sensors use the Surface Plasmon Resonance (SPR) principle which works by the optical excitation at the interface between the metal thin film layer and dielectric layer (or the test sample layer). The most widely used noble metals for the metal layer is gold. Gold has less oxidation and is very resistant to atmospheric contaminants (G. Boisde, A. harmer, 1996). However, gold is very expensive. It has been recently found that copper has better conductivity than gold. It is also cheaper. The main disadvantage of copper is the ease of having oxidation. However, copper is better in term of diffusion. Copper does not diffuse into the silicon substrate when gold does. Copper is therefore used in the standard silicon manufacturing process such as CMOS technology (G.V. Naik, et al., 2013). Furhermore, there is a research result which reports that copper is an excellent plasmonic material (P. Robusto, R. Braunstein, 1981). Also, according to a research work (V.G. Kravets, et al., 2014), the application of Graphene layer over copper layer can significantly reduce the oxidation; thus the copper layer is slowly deteriorated and improves plasmonic characteristic.

Recently, surface plasmon wave find applications in high speed communications and high frequency electronic technology since they have frequencies in the THz ranges (H. Sakai et al., 2016).

The thickness of the metal film has direct effects to the excitation of the surface plasmon wave, both from the consistency of the waves and the amplitudes of the electric fields of the waves. In order to find the optimum waves for the given metal and the given optical source, this project models the excitation using the Kretschmann configuration. We also analyze the result electric field of the surface plasmon wave which take place at the interface between the metal thin film layer and the sample test layer using the finite element method (FEM). We intend to use the economical 632.5 nm red laser light source with thin film copper. The COMSOL

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Multiphysics software (COMSOL Inc., 2017) which supports the FEM is employed.

2 THEORETICAL BACKGROUNDS OF THE SURFACE PLASMON RESONANCE (SPR)

Surface plasmon waves or surface plasmon polaritons (SPPs) are generated at the surface between metal-dielectric interfaces when excited by the incoming light with an appropriate frequency. The excitation of surface plasmon waves can be done by having light beams contact prisms and the phase of the light at the metal-dielectric interface is matched to the phase of the surface plasmon waves. In the early years of the research in this area Otto (Y. Suzuki et al., 1989) and Kretschmann (T.A. Leskova et al., 2000) developed an experimental optical excitation which created SPs waves by using a prism and coated a metal thin film on the surface of the prism. Attenuated total reflection (ATR) is a technique to observe the plasmons. The reflected light intensity are measured by changing the incident angles of the incoming light to various degrees. At a certain angle which is referred as the "resonance angle", the reflected ATRs from the prism signifies the light absorption by the electrons in the metal and their resonance which in turn creates the surface plasmon wave at the metal–dielectric interface. Apart from this, there are also researches which use the grating (A. Iadicicco et al., 2005) and optical waveguides (Wei Du and Feng Zhao, 2014) for the optical excitations of surface plasmons.

The Kretschmann method employs a detecting microscope which moves to different positions to give different angles as shown in Figure 1. When the incoming light travels from the medium which has higher refractive index to the medium which has lesser refractive index, and the light impacts the interface between the two medium with the angle greater than the critical angle, the light will be totally reflected. This phenomenon is called Total Internal Reflection (TIR). The TIR creates a kind of electromagnetic wave between the contact surfaces of the two media called the evanescent electromagnetic field. The minimum amount of the total internal reflection is observed when the incoming energy of the incident light is coupled onto the flat metal. This is referred to as “attenuated total reflection” (ATR).

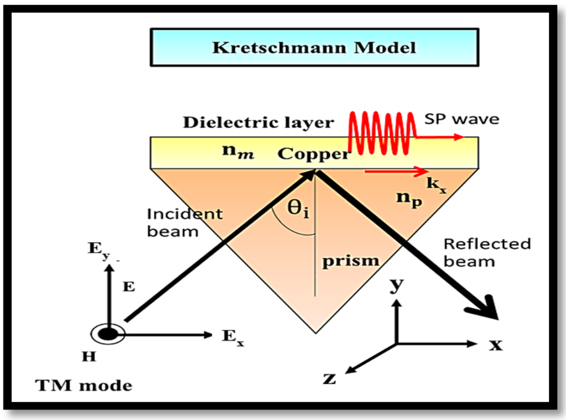

Figure 1: Surface Plasmon excitation at the surface when activated by light impact to the prism using the Kretschmann’s configuration.

As shown in Figure 1, the TM-polarized incident light impacts the prism and activates the excitation of the surface plasmon waves at the interface between the metal thin film and dielectric layer (air layer). The wave vector of the light can be adjusted to be equal to the wave vector of the surface plasmon by launching it from the prism through the metal thin film. The prism is a medium with a higher refractive index than the metal film. Light moving in the prism is reflected at the prism-metal layer interface by means of total internal reflection. The evanescent field of the reflected light at the prism-metal interface penetrates into the metal. With the appropriate thickness of the metal layer, the evanescent wave reaches the metal-dielectric interface (or metal-air interface). In the case that the phase of the incoming light propagating in the prism matches the phase of the surface plasmon waves, the surface plasmon resonance is generated and surface plasmon waves propagate along this metal-dielectric interface. They are generated according to a certain condition which depends on the incident angle and the incident wavelength:

$$k_{sp} = k_x = k_0 n_p \sin\theta \tag{1}$$

k_{sp} is the wave vector of surface plasmon waves
k_x is the wave vector of the incoming light
n_p is the refractive index of the prism
θ is the resonance angle (ATR angle)

According to the equation, the energy and momentum of the incoming light which impact the prism are transfered to the electrons group of the metal thus excites surface plasmon wave. Dispersion relation of surface plasmon wave is shown in the following equation:

$$k_{sp} = k_x = \frac{\omega}{c}\sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}} \quad (2)$$

When the dispersion relation is combined with the excited condition, it is found that the minimum incident angle of the incoming light is:

$$\theta = \sin^{-1}\left(\frac{1}{n_p}\sqrt{\frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d}}\right) \quad (3)$$

If the wavelength of the incident light and the relative permittivity of the metal layer are known, the suitable incident angle which activates the surface plasmon wave can be calculated.

3 THE SIMULATED EXPERIMENTS

The excitation of the surface plasmon resonance phenomenon needs to have the k-vector of the activating light which impacts the prism equals to the k-vector of the surface plasmon wave (SP wave) at the interface between the metal thin film layer and the air layer. We therefore simulate the light activation using the Kretsckmann's configuration which is a relatively easy to implement activation method. A prism with high refractive index and coated with copper thin film is implemented as shown in Figure 2. Electric fields of the surface plasmon wave at the copper-air interface (metal-air interface) are analyzed using the finite element method (FEM). The COMSOL Multiphysics software is deployed.

Parameters as shown in the Table 1 are set according to the dispersion relation. This is to make the k-vector of the p-polarized (TM mode) light which impacts the prism equals to the k-vector of the SP wave. When the light penetrates into the metal thin film, free electrons groups in the metal are coupling with the activating light and vibrate resonantly with the frequency of light. This phenomenon is called the surface plasmon resonance.

When the incident angle of the light is equal to the resonance angle (also called the Attenuated Total Reflection angle θ_{ATR}), the parallel component of k-vector of the incoming light is matched to the parallel k-vector of the surface plasmon. At this stage, the light transfers its energy to electrons groups in the metal and becomes surface plasmon energy. There is no reflect back of the light from the prism. The evanescent wave at the metal-dielectric layer couples to the surface plasmon which results in the propagation of the surface plasmon wave along to the metal-air interface as previously mentioned.

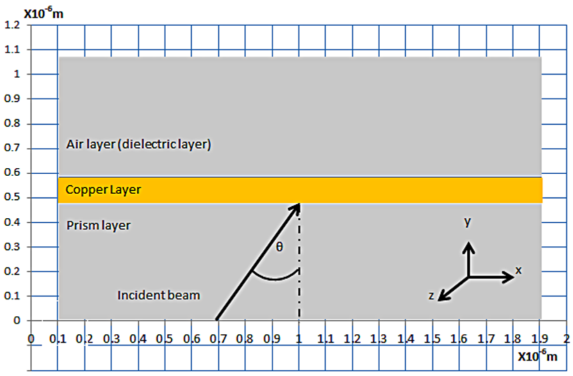

Figure 2: The optical excitation of the Kretschmann's configuration.

Table 1: Important parameters of each medium.

Parameter name	Value
Refractive index of Air	1
Refractive index of Prism (BK7)	1.5151
Relative permittivity of Prism (Real part)	2.2955
Relative permittivity of Prism (Imaginary part)	3.6715e-8
Refractive index of Copper Thin film	0.30730
Relative permittivity of Copper (Real part)	-11.681
Relative permittivity of Copper (Imaginary part)	2.1090
Incident wavelength of Light	632.5 nm
Power of Light	1 W
kx	$k0*n_{prism}*\sin(\theta)$
ky	$k0*n_{prism}*\cos(\theta)$

In this simulation project, the incident angles are changed gradually 1 degree at a time from 30 to 80 degrees. Corresponding surface resonance waves which are activated by the light are observed. The light source is the TM mode laser which has the wavelength of 632.5 nm with a power of 1 W. The simulated thickness of the copper layer varies from 20 nm, 40 nm, 60 nm, 80 nm to 100 nm.

Electromagnetic wave propagation as described by the Maxwell's wave equation (in frequency domain) is as follows:

$$\nabla \times \frac{1}{\mu_r}(\nabla \times E) - k_0^2\left(\varepsilon_r - \frac{j\sigma}{\omega\varepsilon_0}\right)E = 0 \quad (4)$$

where ε_r is the relative permittivity of material

E is the electric field equation

k_0 is the wave vector in free space

It is a differential form equation. We use this equation in the RF module of the Comsol Multiphysics for analyzing the amount of the electromagnetic field at the interface between the thin metal film and the air.

Moreover, we specify Floquet boundary condition both at the left surface and the right surface of every layer in this model to ensure the symmetry of the electric field along and parallel to the interface in the x-y plane.

We also determine the Port boundary condition of this model by using the bottom boundary as Active Port for light impact. The input power of the laser source is set to 1 Watt. The top boundary is used as the Passive Port which allow light to be transmitted through without reflections.

For the meshing of the 2D geometry in this research work, We partition the subdomain into triangular mesh elements. The resolution of the mesh is set to be extra fine.

For the impact angle from 30 to 80 degrees, we use the Parametric Sweep to be range(alpha_min,alpha_step,alpha_max) where alpha_min is equal to 30 degrees, alpha_max is equal to 80 degrees, and alpha_step is 0.01 degrees.

After specifying physical quantities such as material properties, constraints, parameter, COMSOL Multiphysics is then internally compiles all related PDE equations automatically using the finite element analysis. Multiple solvers are used together with adaptive meshing and error control which has been previously specified. Results can be observed from the graphical user interface.

4 RESULTS

In the first analysis using the finite element method on the COMSOL Multiphysics software, the TM-polarized incident light with the 632.5 nm wavelength impacts the prism with different impact angles. We found that when the surface plasmon resonance phenomenon takes place at the interface between the air layer and the copper layer with the thickness of 20 nm, 40 nm, 60 nm, 80 nm, and 100 nm, there are surface plasmon waves when the incident angle of the incoming light is 44.8 degrees. The incident angle and the light's wavelength correspond with the dispersion relation equation. However, the characteristics of the electric field of surface plasmon wave are different when the thickness of the thin copper film layer is changed.

When the surface plasmon resonance phenomenon is taking place at the contact point between the metal thin film and the air, if the thickness of the metal film is suitable, and the impact angle of the TM mode light is suitable, the simulated electric field at the interface will be clearly seen with high amplitude. This demonstrates that the light reflectance approaches the minimum or even zero. Such an angle is called the resonance angle.

The resonance angel can be shifted if the dielectric layer is changed to other materials such as biomolegular sustances. The resonance angle is therefore can be applied to checked the existence of bio-molecular DNA.

When the copper thin film thickness is 20 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The average amplitude is 5.1×10^4 V/m as shown in Figure 3. The electric field that occurs does not show clear patterns and does not seem to be consistent along the copper-air interface.

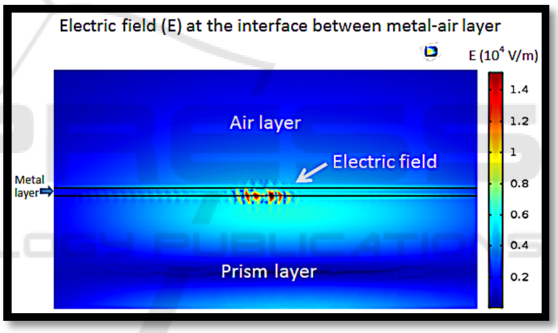

Figure 3: Electric fields of surface plasmon wave at the interface between the 20 nm copper film and the air.

When the copper thin film thickness is 40 nm, it is found that the electric field between the copper-air interface has high amplitudes. The average amplitude is 2.7×10^5 V/m as shown in Figure 4. The

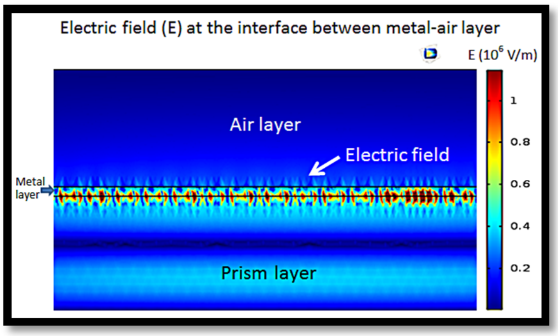

Figure 4: Electric fields of surface plasmon wave at the interface between the 40 nm copper film and the air.

electric field that occurs show clearer patterns and consistent along the copper-air interface.

When the copper thin film thickness is 60 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The average amplitude is 2.2×10^4 V/m as shown in Figure 5. The electric field that occurs show unclear patterns and not consistent along the copper-air interface.

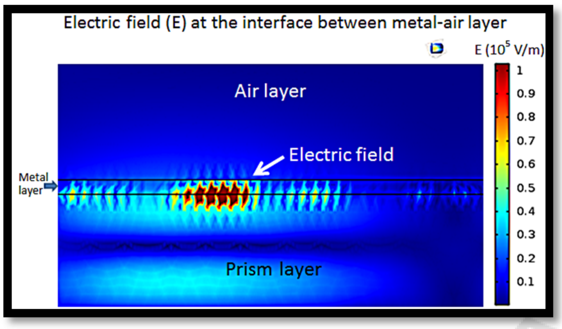

Figure 5: Electric fields of surface plasmon wave at the interface between the 60 nm copper film and the air.

When the copper thin film thickness is 80 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The average amplitude is 2.9×10^4 V/m as shown in Figure 6. The electric field that occurs show unclear patterns and not consistent along the copper-air interface.

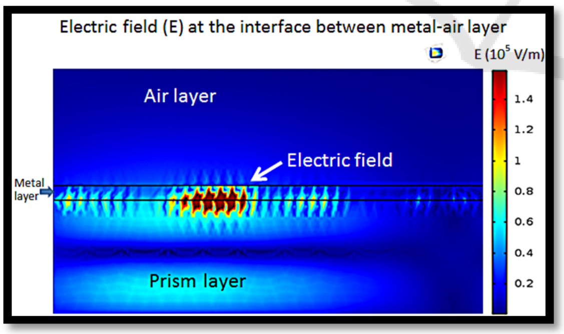

Figure 6: Electric fields of surface plasmon wave at the interface between the 80 nm copper film and the air.

When the copper thin film thickness is 100 nm, it is found that the electric field between the interface of the copper film and the air still has very low amplitudes. The average amplitude is 1.1×10^4 V/m as shown in Figure 7. However, the electric field that occurs does not show clear patterns and is not consistent along the copper-air interface. The patterns can not be used to identify if they are surface plasmon wave at the interface.

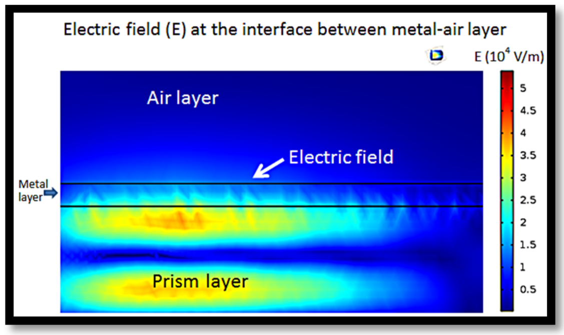

Figure 7: Electric fields of surface plasmon wave at the interface between the 100 nm copper film and the air.

A graph is plotted to show the relationship between the maximum amplitude of the electric field at the copper-air interface and the thickness of the copper film. The graph shows a concave downward pattern. The highest point of the graph is when the thickness of the copper film is 40 nm. This is the best point when activated by the 632.5 nm light source.

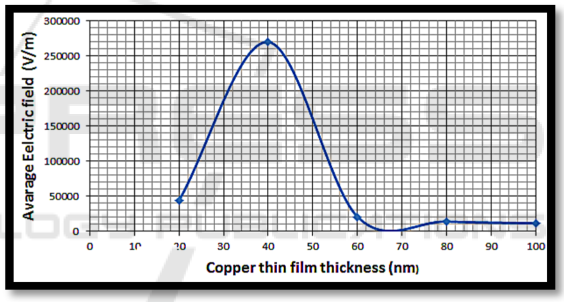

Figure 8: The graph which shows relationships between the maximum amplitude of the electric field at the copper-air interface and the thickness of the copper thin film.

The next step is to find the most suitable impact angle for the given light source. We then change the impact angle parameter to other values around the 44.80 degrees (this is the degree according to the dispersion relation equation) and keep the impact light TM mode to have the wavelength of 632.5 nm to find a suitable impact angle for best surface plasmon resonance phenomenon. The simulated observable surface plasmon wave with highest amplitude at the interface between the copper thin film and the air are considered. Table 2 shows the observation results.

After having the first results, the second analysis is conducted. The finite element method on the COMSOL Multiphysics software is still employed. The wavelength of the TM-polarized incident light is changed to be 785 nm with a power of 1 W and the incident angle is now changed to be 44 degrees. The thickness of the thin copper film are 20 nm, 40 nm, 60 nm, and 80 nm. The simulated electric field patterns and amplitudes are observed.

Table 2: The incident angles (Θ_{ATR}) which are suitable for different copper thin film thickness.

Copper thin film thickness (nm)	Optimized incident angle (Θ_{ATR}, degrees)	$\Delta\Theta$ (degrees)	E_{avg} (V/m)
20	44.14	0.66	4.4×10^4
40	44.80	0	2.7×10^5
60	44.84	0.04	2.1×10^4
80	44.86	0.06	1.4×10^4
100	45.88	1.08	1.2×10^5

When the copper thin film thickness is 20 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The average amplitude is 2.8×10^4 V/m as shown in Figure 9. The electric field that occurs show clear patterns and consistent along the copper-air interface.

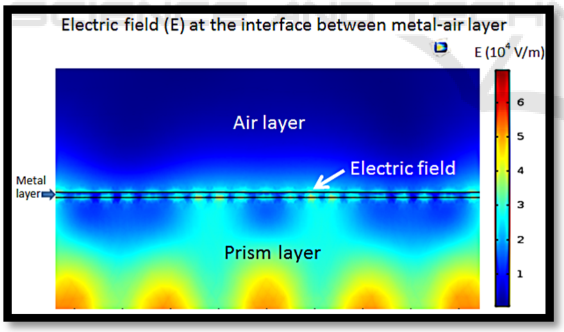

Figure 9: Electric fields at the interface between the 20 nm copper film and the air when the light has 785 nm wavelength.

When the copper thin film thickness is 40 nm, it is found that the electric field between the interface of the copper film and the air has high amplitudes. The average amplitude is 2.5×10^5 V/m as shown in Figure 10. The electric field that occurs show clear patterns and consistent along the copper-air interface.

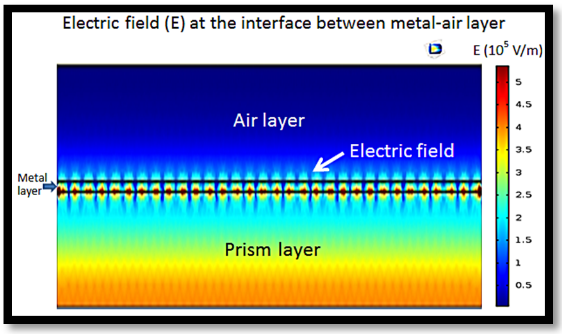

Figure 10: Electric fields at the interface between the 40 nm copper film and the air when the light has 785 nm wavelength.

When the copper thin film thickness is 60 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The average amplitude is 2.5×10^4 V/m as shown in Figure 11. The electric field that occurs show unclear patterns and not consistent along the copper-air interface.

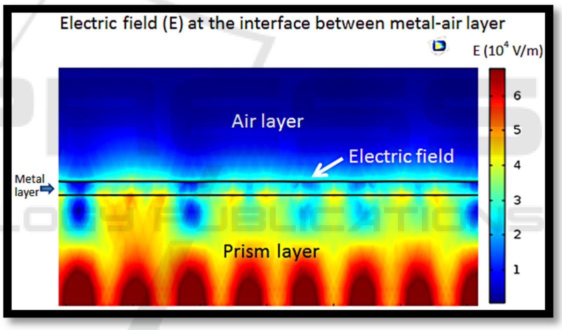

Figure 11: Electric fields at the interface between the 60 nm copper film and the air when the light has 785 nm wavelength.

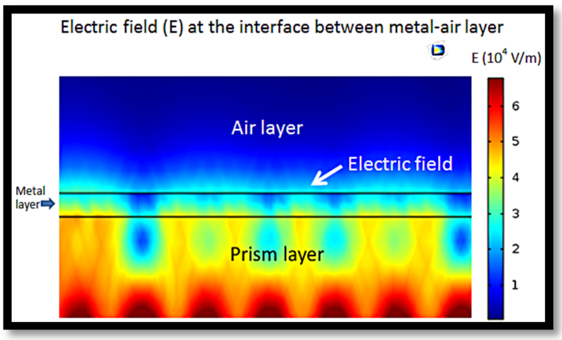

Figure 12: Electric fields at the interface between the 80 nm copper film and the air when the light has 785 nm wavelength.

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When the copper thin film thickness is 80 nm, it is found that the electric field between the interface of the copper film and the air has low amplitudes. The maximum amplitude is 2.7×10^4 V/m as shown in Figure 12. The electric field that occurs show unclear patterns and not consistent along the copper-air interface.

From the simulation results, it is found that the thickness of the thin copper film has direct effect to the occurrence of the surface plasmon waves. The thickness of 40 nm is considered the best thickness for the activation with the 632.5 nm wavelength. It yields very clear and consistent surface plasmon waves pattern. It also has the highest electric field amplitude at the copper-air interface.

Our analysis results which are obtained by using the finite element method, give similar results to (F. Atida Said et al., 2016) which uses the finite difference method when the incident light source has 785 nm wavelength. That is, when the light source with the 785 nm wavelength is used, the best copper thin film thickness is 40 nm. It gives high and consistent surface plasmon wave amplitudes at the copper-air interface.

5 CONCLUSIONS

Recently, researches in the area of plasmonics have been highly active. There are applications in various areas such as biomedical engineering where SPR devices are used as sensors to detect the presence of DNA molecules which are adhered to metal surfaces. Such adhesion layer change the local refractive index which results in the shift of the resonance angle of the incoming light. Moreover, the electric field of the plasmon wave with high applitudes can be used to generate second (or third) harmonics due to surface plasmon coupling (E.M. Kim et al., 2005) (H.J. Simon et al., 1974). This could identify the structural information of bio-molecular substances. Plasmons also have been considered as a means of transmitting information on computer chips. This is another potential application in technology. Plasmons support frequencies in the THz range. This would solve the data loss problem of conventional wires which have the GHz transmissions loss problem. In this project, we try to find the suitable thickness of the copper film which creates the surface plasmon resonance at the copper-air interface when the light source is the 632.5 nm TM mode. This light source is an economical red laser which can be easily found commercially. It is cheaper and easier to find than the green laser and blue laser lights. Based on the finite element method, the results suggest that the copper thin film with the thickness of 40 nm is the most suitable one for the surface plasmon resonance using the Kretschmann configuration. The simulated electric field amplitude at the copper-air interface is high and consistent along the interface when the 632.5 light is applied which also means that the best surface plasmon resonance is generated at this metal-air interface. It is very likely that if a Graphene film is applied over the copper thin film with the thickness of 40 nm, the plasmonic characteristics will be positively improved; thus improves the copper based surface plasmon sensors which are to be developed.

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