Structural Characteristics of Au-GaAs Nanostructures for Increased Plasmonic Optical Enhancement

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ABSTRACT

This research has been performed to improve upon optical qualities exhibited by metallic-semiconductor nanostructures in terms of their ability to excite electrons and generate current through the fabricated device. Plasmonic interactions become very influential at this scale, and can play an important role in the generation of photocurrent throughout the semiconductor. When the device is fabricated to promote the coupling of these radiated electromagnetic fields, a very substantial optical enhancement becomes evident. A GaAs substrate with an array of Au nanowires attached to the surface is studied to determine structural qualities that promote this enhancement. Using computational electromagnetic modeling and analysis, the effect of the Ti adhesion layer and various structural qualities are analyzed to promote photocurrent generation. Emphasis is placed on the amount of enhancement occurring in the semiconductor layer of the model. The photocurrent is then calculated mathematically and generalized for optimization of the device.

Keywords: Plasmonics, surface plasmon, optical enhancement, photocurrent, nanowire, photovoltaic.

1. INTRODUCTION

Metallic structures (Au for this work) have long been known to be efficient conductors of electricity. This is due to the loosely bound electrons that exist in the metal. Appling an electric field across the metal will cause a current to flow through the material. Photonics is generally described as the study of light, in which light is comprised of an alternating electric and magnetic field propagating through a medium. This electromagnetic field has a periodic nature and has an associated wavelength with it. To combine the nature of the metal and the incident light, the study of plasmonics is formed. More specifically, plasmonics "is based on interaction processes between electromagnetic radiation and conduction electrons at metallic interfaces or in small nanostructures, leading to an enhanced optical near field of sub-wavelength dimension."[1] The electric component of the incident electromagnetic field reaches the metallic surface, and the free electrons in the metal begin to oscillate collectively to form surface plasmons. These surface plasmons are bound to the surface of the metal, and have exponentially decaying electromagnetic fields.[2]

The importance of plasmonics becomes apparent at the nanoscale, as structures may be *tuned* to use this optical enhancement to make a more efficient device. Sensing and photovoltaic devices currently use this principle to construct microscale and nanoscale devices that are effective performers. This has led to much research in the areas of structure geometry and fabrication to determine optimal qualities that will generate maximum enhancement. Common geometries include the nanowire and nanotoriod arrays, as these structures can be accurately modeled and fabricated.[3,4] The nanowire geometry will be of primary focus in this paper and plasmonic enhancement will be shown and calculated using computational electromagnetic software.

This work studies their ability to generate current in the adjacent semiconductor layer. The radiated electromagnetic field that is generated from surface plasmons in the metal can effectively collect at a specified point in the structure, and this can be used to generate enhancement in the semiconductor. By careful study of the geometry, it can be shown that it is capable to influence the photocurrent created by the device. Prior studies on the microscale have shown that an array of interdigital Au electrodes performs as a very efficient photodetection device.[5,6] This array of microscale Au wires has

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been fabricated and tested to show significant photocurrent generation in the GaAs.[5] Due to the dimensions of the structure being on the microscale, the plasmonic effects are minimal as compared to the nanoscale. Furthermore, nanostructures also tend to have much greater enhancement in the gap due to the plasmonic coupling that occurs at this scale. By fabricating the metallic structures closer together (reduction to nanogaps), the plasmonic resonance is shown to be stronger as the structures approach one another.[3]

The materials and geometry of this structure were predefined from prior work and modifications were made to the model to generate an extension of this research to the nanoscale.[5,6] Various structural qualities are modified to attempt to generate the maximum optical enhancement occurring in the GaAs substrate layer of the model, emphasizing the additional generation of photocurrent in the device. Dependent on the intentions of the device, analysis of the geometry and materials of the structure will lead to more enhanced, efficient photoelectric devices.

2. RESEARCH GOALS

The primary goal of this research is to expand on modern research in the field of nano-optics and attempt to computationally characterize geometries of interest in terms of optical enhancement and photocurrent generation. Nanoplasmonic applications have become very relevant not only in academic research, but industrial applications as well. Due to the general ability for these devices to increase the electromagnetic fields received from light, they prove to be appropriate structures for many photovoltaic and photodetection applications. It is necessary to understand that different geometries create different effects throughout structure, and nanoscale dimensions pose certain problems in terms of fabrication. This work focuses on a specified geometry and plasmonic hotspot analysis. It is intended to show that careful analysis and fabrication of metallic-semiconductor devices (more specifically Au-GaAs) can lead to greatly increased optical enhancement quantities due to plasmonic effects.

3. DESCRIPTION OF EXPERIMENT

Due to the limitations and expenses involved with the fabrication of nanostructures, it is necessary to use more efficient methods to analyze their properties. Computational electromagnetics provides this information to the researcher via software tools that can accurately model and compute data as specified by the user. COMSOL Multiphysics® is a software tool used for finite element method (FEM) modeling and analysis of a variety of structures. Further discussion regarding model properties follows in the next section of this report.

After the model is verified for accuracy, structural characteristics of the geometry are modified to determine the amount of optical enhancement reaching the substrate layer. The three major portions of this research involve parametric sweeps of the (1) titanium adhesion layer, (2) width and array spacing of the Au nanowires, and (3) the thickness of the Au nanowire. Each parameter will be shown to have an optimal dimension, and in combination will result in conclusions about an optimal device structure.

4. MODEL PROPERTIES

The model used consisted of a modified geometry that was used in prior work.[5,6] This resulted in a model that exhibited nanoscale dimensions in terms of structural width, thickness, and spacing. Other than modeling the structure itself, it is necessary to format the environment space to ensure it simulates as close as possible to an actual physical environment. The model was enclosed vertically by two perfectly matched layers (PMLs) to ensure that all scattered light from the device did not reflect back into the simulation space and affect calculations. These layers are used to absorb the scattered electromagnetic radiation. Below the upper PML is a layer of air that is modeled with a height of three times the wavelength of the incident light. Additionally, the Au-Ti structure is modeled on top of a GaAs layer that extends down to the bottom PML. The left and right edges of the model were applied with a periodic condition, to generate an infinite array of the nanostructures in the x-direction. From the top of the model, light with a wavelength of 875nm is simulated and normalized to a magnitude of one for simplicity of enhancement calculations. The electric component of this light (E_0) is what generates the plasmonic excitation on the surface of the metal, and it is polarized along the width of the Au nanowire as indicated in Figure 1a. Materials in the geometry were defined using interpolation tables that generate the index of refraction as a function of wavelength. Each portion of the geometry was applied with the appropriate material properties, and each layer corresponds to a different material. A fillet of 5nm was also applied to the upper portions of the Au geometry to model the true geometric result of the nanofabrication process. Figure 1a shows an annotated representation of the model, which is viewed as a cross section in the x-y plane. The two-dimensional representation of the devices assumes z-dimensions of infinity. Figure 1c also provides a graphical representation of the model; the actual height ratio of the Ti and Au are not to scale. The overall model creates an infinite array of Au-Ti-GaAs structures with infinite lengths in and out of the page.

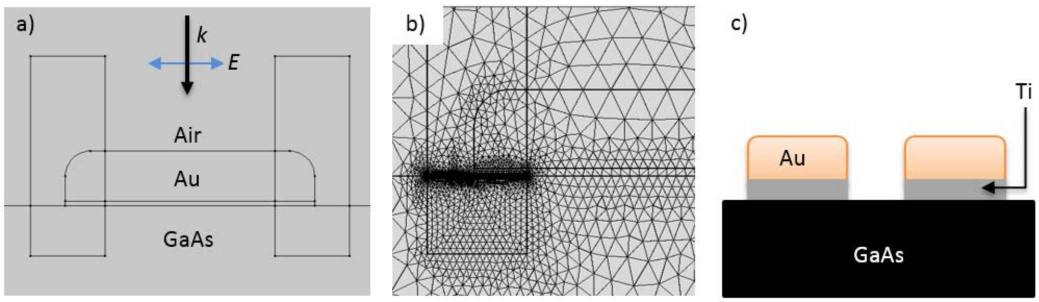

Figure 1. a) Annotated image of FEM model. Ti layer is modeled as thin layer between Au and GaAs geometries. Rectangular integration areas are shown on left and right edges. b) Model after mesh has been applied. Area shown is general region of plasmonic enhancement, and contains a minimum 10 nm mesh size. c) 2D representation of model with materials labeled.

Two rectangular geometries, occurring on either side of the Au structure, were created for accuracy during analysis of the device. The plasmonic hotspot will be shown to occur at the lower regions of the metal, where it forms an interface with the GaAs. These rectangles are used to create a finer mesh in this area of the model, and the box that is formed in the GaAs region is used as an integration area during analysis of the Ti adhesion layer. Meshing the model creates a number of data points throughout the geometry. It was found that creating a finer mesh (~10 nm) proved to provide the most accurate results, and this was used primarily in the region where the hotspot is located. Figure 1b shows a detailed image of the mesh created in this integration area. Due to the exponential increase of simulation run-time with smaller meshes, the hotspot and GaAs regions were the only two areas where this dimension of mesh was applied. This technique allowed for fairly rapid simulation of the model. Data in this report is collected and defined as a surface integration over a defined area of the model. The results section will provide information on the area of integration used for each particular study.

5. EXPERIMENTAL RESULTS AND CONCLUSIONS

The experiments performed for this research are generated for the goal of generation of maximum optical enhancement in the GaAs layer of the model. By varying the adhesive layer and structural characteristics of the model, this is achieved and shown using graphical and mathematical representations. This section is broken down into two parts, (i) effects of Ti adhesion layer and (ii) structural characteristics. Both describe the results achieved along with a description of the reason why these are accurate and reasonable.

(i) Effects of Ti adhesion layer

Due to material properties, many metal-semiconductor interfaces need some form of adhesion to ensure that the metal stays attached to the surface of the semiconductor. Commonly, Ti, Cr, or other metallic variations are used as the adhesive.[7] Nanofabrication techniques usually deposit a semi-uniform layer of the adhesive material prior to deposition of the metal to ensure that the metal will stay adhered to the semiconductor. This is an important part of fabrication, and it is necessary to ensure optimal device performance. Although usually necessary it has been shown that this layer produces "damping" effects of the plasmonic enhancement that occurs on the structure.[7] Increasing the Ti layer proves to not only move the hotspot away from the GaAs, but also reduce the magnitude of the plasmonic resonance that occurs from the incident light. It also is possible to fabricate Au-GaAs interfaces without an adhesion layer. This is represented throughout the Structural Characteristics of this report to simplify the model.

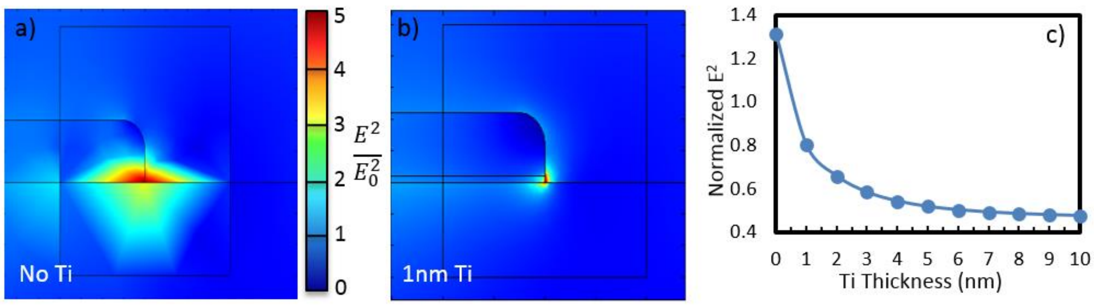

Figure 2. a,b) Optical enhancement shown at plasmonic hotspot of structure. Evident that enhancement is greatly increased due to total removal of Ti layer. c) Plot showing numerical analysis of enhancement as a function of Ti thickness. Data plotted was received from inside the integration rectangle only in the GaAs.

Numerical analysis is performed by integrating over the portion of the integration rectangle that exists in the GaAs region for all values of Ti thickness. This is done to ensure that the optical enhancement that is generated by reduction of this layer was the primary focus of the study. The thickness of the Ti is swept from 10nm to 1nm, then totally removed from the model. The plot in Figure 2c shows the mathematical representation of the normalized enhancement in this area as a function of this reduction. Clearly total removal of the Ti generates a significant increase in enhancement. Due to this, the remainder of the experiments is performed with a geometry that does not include the Ti layer.

(ii) Structural characteristics

Optical analysis of the Ti layer carries similarities to examining other properties of the structure. Being an array of electrodes, each Au nanowire has three dimensions that may be varied. These parameters include electrode spacing, width, and thickness. As each parameter is varied, optical enhancement is calculated and used for additional photocurrent calculations.[5] See Figure 3c for a detailed representation of the modified parameters and their appropriate notations. Spacing (*s*) and width (w) are initially used to model the nanogap and nanowire width. Both of these variables are swept across a nanometer range that corresponds to current fabrication allowances. As expected, it is shown that by decreasing the gap (*s*), optical enhancement increases due to coupling of the electromagnetic fields produced by plasmonic effects. The width of the wire also shows to play a small role in photocurrent generation, and this is a topic of future study within the model. Regardless of the effects the width may have, spacing proves to be the more important variable in terms of optical enhancement. Figure 3a shows that a 5 nm increase in structure spacing reduces the enhancement recorded in the GaAs by approximately 50%.

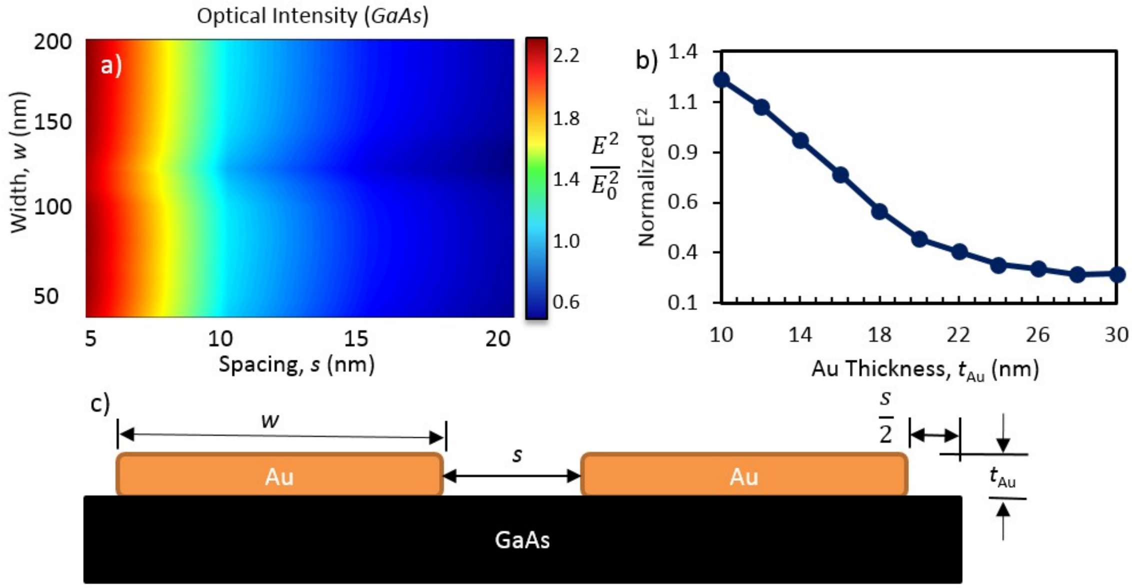

Figure 3. a) Optical intensity plotted as a function of width and spacing of the geometry. b) Optical enhancement over entire GaAs layer due to thickness variations of Au. Note values are normalized for simplicity. c) Graphical representation of variables included in model.

Following analysis of the width and spacing of the device, the thickness of the Au (t_{Au}) is studied. Similarly to the prior analysis, this dimension is swept through nanometer values within an applicable region. This region corresponded from thickness values of 10-30 nm. It is found that by decreasing the thickness of the metal, more enhancement is generated in the GaAs layer. This corresponds directly to an increase in photocurrent throughout the device. During this portion of simulation, data is derived from the entire GaAs region rather than only the hotspot area. This is due to the dependency of photocurrent calculation on an integration of the data across this entire substrate region. While the hotspot of the plasmonic effect is an important study, it is more relevant to determine the amount of current that the device is able to generate. Overall conclusions regarding an optimal structure imply a geometry with a minimal electrode spacing and Au thickness.

6. FUTURE SUGGESTED RESEARCH

The research performed in combination with prior research confirms that reduction of the adhesion layer between the metal and semiconductor creates a significant device performance in terms of photocurrent generation.[7] Computationally it was verified that entire removal of this layer is the most effective method of increasing optical enhancement in the GaAs layer. Future research involving different adhesive materials and fabrication techniques could lead to devices that eliminate the poor effects that an adhesion layer exhibits. Also, different substrate materials have the potential to exhibit qualities that allow metallic structures to adhere soundly without the presence of an adhesion layer. The combination of efficient metal-semiconductor compounds and no additional layers would provide for a significantly enhanced photocurrent generator.

Computational electromagnetic software is a very effective tool for efficient testing and design of theoretical devices. Recently, a variety of software has been accepted as accurate in terms of consideration of data, and many studies use this method. Where it does provide ease and general reliability, it lacks absolute accuracy. Some physical concepts are not currently able to be simulated in software, and generalities about materials and environments must be assumed. Also, fabrication currently does not allow for perfect surface smoothness precision and fabricated devices will not be exact representations of the geometries that are being modeled. However, for the most part, computational model have been shown to be very accurate for predicting electromagnetic results. The thickness of the metallic layer studied proved to be a significant player in terms of device efficiency. Preliminary experimental data agrees with these conclusions but more accurate results could potentially be realized using a three-dimensional representation of the structure. As previously mentioned, infinite quantities were modeled for distance in the z-direction and the length of the periodic array in the x-direction. Also, it is important to consider the electrical properties of the device. Future work will investigate this, where this work focuses on the optical characteristics of this structure.

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