Design of Asymmetrical Grating Couplers for Surface Plasmon Enhanced Illuminators Through Rigorous Computer Simulation

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Abstract

Finite difference time domain electromagnetic simulation of asymmetrical grating structures is used to identify promising plasmon enhanced illuminators (PEI). Such PEIs have important applications in microscopy, surface enhanced Raman scattering, and even heat-assisted magnetic recording. The design of PEIs is complicated by the need for directional coupling and low re-radiation of previously coupled energy. Computer simulation can guide this technology development by giving insight to the physical interaction and quantitative coupling coefficients. Our approach is to use finite-difference time domain analysis to explore coupling efficiency as a two step process. The first step is the characterization of the scattering from collection elements. The second step is to combine elements using a signal flow graph based on two port models. Of particular interest are asymmetrical elements that in addition to providing directional coupling, also allow low re-radiation. Ultimately, through this approach we aim to increase the local electric field transmission by a factor of 1,000 for surface plasmon enhanced Raman scattering. The two step process will be verified by direct computation of the full grating geometry.

1. Introduction

By nature, surface plasmons polaritons (SPP) exist in the form of freely moving electrons oscillating in resonance with a time-varying electromagnetic field (such as a plane wave) at the surface of a conducting medium. Surface plasmons play an important role in optical based circuitry as they can allow light to be transmitted into a sub-wavelength aperture or waveguide which provide important applications in scanning optical microscopy (SOM), Raman Spectroscopy, photovoltaic devices, as well as other sensor based technologies. However, numerous challenges arise when it comes coupling such surface plasmons from an incident plane wave. For instance, in the case of a 700nm plane wave incident to a silver conducting plane, no plasmon will be excited within the conducting surface. Due to the high
refractive index of silver, or any other conductor for that matter, the incident plane wave will be reflected back from the direction it came. Therefore, in order to provide maximum coupling, the use of a corrugated surface such as a grating must be applied in order to disperse the incident light and provide maximum plasmon coupling along the conducting surface. A simple graphic of structure can be seen in the diagram:

Figure 1(Left): The physical structure of an asymmetrical geometry grating with 4 elements. The blue structure is the silver substrate to which we are attempting to couple plasmons.

Figure 1(Right): Cross section of a single grating structure as it is set up in TEMPEST. Each grating is roughly 700nm in width. The separated distance of each grating from the substrate in simulation is close to 200nm.

Here we seek to explore the application of various asymmetric plasmon grating coupler topographies and analyze their effects on coupling efficiency, transmission and ultimately examine the total plasmon output from a multi element grating. Our analysis of grating structures will be verified by the use of a finite difference time domain simulator called TEMPEST which models Maxwell’s equations to simulate the effects of electromagnetic fields on surface plasmons on a conducting plane. Due to the computational complexity of such simulations we will be analyzing each grating structure as a two dimensional cross section which can easily be extended to third dimension. The design of surface plasmon grating couplers is greatly complicated by the presence numerous design parameters and physical quantities that affect the total plasmon output from a given grating coupler geometry. Therefore, each grating structure must be analyzed on a case by case basis to find the optimal geometry. Many such simulations have been run and in our discussion we will only discuss those of particular interest.
2. Single Element Gratings and their Extension to a Multiple Element Grating

When examining plane-wave to plasmon interaction from a single grating element it is important to quantify various physical quantities such as the directional coupling efficiency, transmission, and ohmic losses that occur as the energy of the plane wave is transferred to a surface plasmon. When considering plane wave to surface plasmon coupling there two variables that need to be considered: plasmon coupling to the right as a function of illumination angle, which we will call \( C_R(\theta) \) and plasmon coupling to the left which will be denoted by \( C_L(\theta) \). The plasmon coupling in a given direction varies greatly by illumination angle, therefore, it is important to describe how much plasmon is coupled at a given angle by generating a polar plot for each the leftward plasmon coupling as well as the rightward plasmon coupling. For instance the fin structure in the preceding section gives the following antenna plot:

![Polar Plot Example](image)

*Figure 2:* To determine the plasmon output from a given illumination we run 17 independent simulations from -80° to +80° in intervals of 10° and measure the coupled plasmon from each angle. The scattered field from a -30° angle can be seen in the figure to the right.

In addition to plane wave to plasmon coupling, plasmon transmission must also be considered. Transmission is defined as how much coupled plasmon energy is able to be transmitted past each neighboring grating structure. A higher transmission coefficient indicates that a plasmon travelling along
the substrate is not reradiated as it reaches a grating. From the previous diagram, it should be clear that a single element grating behaves almost as a “black box.” The incident plane wave can be thought of as an input to the system and the resulting left and right surface plasmons can be considered the resulting outputs from the system. In a multiple element system, the output from a given grating is a sum of the coupled plane wave plasmon plus the transmitted plasmon from every grating structure before it. This sum can be quantified as follow.

\[
b_{nR} = r a_{nR} + t a_{nL} + c_R(\theta) \sqrt{S_{inc}} e^{j k\sin(\theta) P_n}
\]

\[
b_{nL} = r a_{nR} + t a_{nL} + c_L(\theta) \sqrt{S_{inc}} e^{j k\sin(\theta) P_n}
\]

Here \( b \) is the total output at a particular grating in either direction, \( r \) is the reflection coefficient, \( t \) is the transmission coefficient, \( C(\theta) \) is the coupling equation \( S_{inc} \) is the plane wave Poynting vector and the complex exponential term describes the phasor propagation of the plane wave. Using this model allows us to expand the output from a single element grating to a multiple element grating through the use of a signal flow graph which can ultimately be solved via an inverted matrix in Matlab.

**Figure 3 (Signal Flow Model):** Each grating element can be considered as a node within a signal flow graph. The inputs to each element include the energy of the incident plane wave as well as the transmitted energy from the grating before it and also the reflected plasmon energy from the grating in front of it. Combining these variables allows us to extend the output from a single element to a grating structure of many elements.
The signal flow model was verified by a comparison of a full grating simulation to that which was generated by the signal flow model. This simplified signal-flow model is extremely beneficial in terms of computation since one simulation of a single grating can be extended to any number of gratings. The coupling efficiency is best modeled by comparing the plasmon output power to the magnitude of the plane wave’s Poynting vector. Mathematically this can be represented by the following equation:

\[ \sigma = \frac{P_{SPP}}{S_{inc}} \]

Since plasmon power is represented by the units Watts/m and the Poynting vector has units of W/m², we are left with units of meters, however, in our context nanometers and micrometers are more appropriate and will be used from this point forward.

Figure 3 (Signal Flow Model):  Plasmon output data from signal flow graph. On the left, the plasmon output as function of pitch for six elements is plotted. The high peaks are a consequence of a resonant condition where the plasmon output is high due to constructive wave interaction between elements. The second peak is lower due to ohmic resistance. The right graph shows Plasmon output as a function of the number of grating elements present. As we add each grating element the total collective plasmon output increases, however, it reaches an upper bound around 30 elements due to ohmic and radiation losses.

3. Analysis of Coupling Efficiency vs. Transmission
Based upon the signal flow model, it should be clear that the two most important aspects to generating a high plasmon output are the coupling efficiency and transmission between elements. If a particular grating element couples well and has 100% transmission then each added grating element will contribute to the total surface plasmon output via superposition. Unfortunately, due to the principle of reciprocity, the two quantities have an inverse relationship, that is, structures with high transmission generally have low coupling and structures with high coupling in general have low transmission. The issue is further complicated by the fact that larger structures, which generally couple well, are affected more by ohmic losses since the plasmons have a slightly larger distance to travel around the structure. To demonstrate this inverse relationship, consider an angled thin-film grating structure as its width is gradually increased in increments of 60nm, which is less than 1/10th of a wavelength.

\[
\sigma = \frac{P_{SPP}}{S_{ik}}
\]

**Figure 5:** The relationship between cross section (sigma) and transmission as the width of the thin film structure is increased. Overall, there is an inverse relationship between cross-section (coupling) and transmission. At resonance the structure couples well, but has a minimal transmission as it causes much of the plasmon to be radiated.

As expected, with each incremental increase in width, the cross-section of the surface plasmon increases by a nearly proportional amount. Conversely, the transmission amount shows a more irregular trend. At some widths, such as the 300nm width, there is a very low transmission at around 3%. This is most likely due to a resonance condition present in the thin film. At a width of 300nm the film has a
total length of 300nm*sqrt(2) = \textbf{424nm} since it is angled at 45 degrees. A low transmission percentage indicates that this length of film is reradiating almost all of the surface plasmon that reaches it. However, due to reciprocity, this particular structure will also have high plane wave to surface plasmon coupling efficiency. Ideally, we want to achieve an optimal balance between transmission and coupling. In our experience, the most ideal elements are those that have a high transmission with reasonably high coupling as well. So far, this balance is most effectively achieved through elements approximately 600-700nm in width separated around 400nm from the conducting substrate. For instance, in a recent simulation, a 600nm wide thin film structure provided a 16 micron output over 20 elements. Optimal trade-offs of transmission vs. cross-section may vary depending on the topography of element used.

5. Effect of a small gap on surface plasmon coupling

A particularly interesting effect discovered recently with multi-element structures is the effect of thin gaps on the direction of plasmon output. In one simulation we created an asymmetric wing like structure roughly 600nm in width. In a second simulation we used the exact same topography, only differing by a narrow, 15nm gap roughly in the middle of the fin structure. A demonstration of these topographies and resulting plasmon output is given in the following figure:
Figure 6: Note the shift in asymmetry between the structure with the gap compared to the structure without the gap. The left structure (with gap) shows a high amount of leftward plasmon output at the 20 degree angle which is parallel to the direction of the gap. This demonstrates that that gap is able to act as an waveguide coupling energy incoming to the gap. Also worth noting is the fact that the output lobes occur at very similar angles in each simulation.

An interesting consequence of the introduction of this gap is a reversal of the surface plasmon output. As can be seen in the figure, the shape without a gap shows high rightward plasmon output around a -30 degree illumination angle. However, with the introduction of a gap the magnitude of the lobes in the polar plot are reversed. Rather than sending having a maximum rightward output at -30 degrees, there is a high leftward output at around a 20 degree illumination angle. It is also worth pointing out that the locations and shapes of the output lobes do not change with the introduction of the gap, the only significant difference between the two polar plots is at which angle the maximum plasmon outputs occur. The effect of this output reversal can be explained by the fact that the gap acts as a waveguide. If the illumination angle were at 20 degrees than the polarization of the electric field will be orthogonal to the direction of the gap. Since the gap is capacitive it causes a high amount of coupling of the electric field. To demonstrate this, the electric field intensity in the x-direction (left to right) has been magnified in the previous figure. The waveguide effect of the introduced gap may have promising results in the design of grating structures due to the fact that it can be used as a design parameter to shift the receptive illumination angle.
6. Thin film Grating Structures

While insertion of a gap into a grating element shows interesting results and provides insight into the physical interaction of a plane wave with a grating coupler, the most promising results thus far have been from thin film grating structures. That is not to say that thin films are the most optimal geometry, however, they have provided the best results out of what we have tried so far. A brief overview of the results from thin film topographies was given in section four and so far the best result to date has come from a thin film geometry of 600nm in projected width which gives a physical length of approximately 848nm. The signal flow model showed a maximum plasmon output of 16um with X elements at an optimal pitch of around 1.8 microns as shown in figure 4. The maximum rightward plasmon output occurs at a 50 degree illumination angle which is close to the film’s orientation of 45 degrees. The structure also showed a high rightward plasmon output at an illumination angle of 0 degrees. This shows that the structure can act much like a mirror by reflecting the incident light upon the surface of the grating.

![Figure 7: A thin film of 300nm in width (454nm long) shows a high degree of resonance when illuminated from a 50 degree angle. The near fields of the magnetic field of the surface plasmon travelling within the structure can be seen in the above TEMPEST simulation.](image)

7. Observations
As previously stated, analysis of such grating structures is convoluted by the presence of many design parameters and their complicated relationship to the various physical quantities that ultimately determine the plasmon output from a multi-element grating. Even with a solid understanding of electromagnetism, it is difficult to predict exactly how plane wave to surface plasmon coupling will occur. As one could imagine, there are an infinite number of topographies that could be used to design a grating structure, therefore, selecting the optimal structure is difficult task. All simulations have shown that even subtle changes in a single aspect of a grating produce widely differing results in the plasmon output. However, after running several independent simulations some trends have occurred which are worth noting. Most noticeable are the effects of the physical size of the grating structure and its relationship to the plasmon cross section. As mentioned earlier, increasing the physical width of the grating also increases the plasmon output as it gives the plasmon travelling along the grating structure a greater distance to couple to the conducting plane. In our simulations, we saw a large variation on surface plasmon output as a function of grating width, varying anywhere from 20% of the physical width of the grating to as high as almost 175% of the physical grating width. The grating structure showed an optimal physical width at around \( \frac{3}{4} \) of a wavelength or roughly 500nm. In addition, increases the physical distance of the structure from the conducting substrate also increase the transmission by a nearly proportional amount. Based upon these facts, it seems as though optimizing the plasmon output varies greatly on finding proper balance between the physical width of an object and its distance from the conducting substrate.

8. Conclusions and Further Direction

Our primary assumption, that asymmetric grating structures would provide a greater grating plasmon output, did not show to be as promising as expected based upon the data from our simulations. The motivating factor for studying such asymmetrical structures was that they may increase directional coupling while also increasing directional transmission. Although asymmetric objects did in fact increase directional coupling as expected (most notably through the thin film structures), they showed little difference from the symmetrical objects in terms of transmission. Transmission has been shown to be one of the most important factors in generating high collective plasmon outputs since it gives the
plasmon travelling along the conducting surface an opportunity to sneak past each subsequent grating without being reradiated back into space. One of the largest caveats to designing effective plasmon grating couplers is minimizing loss of coupled plasmon energy either through ohmic or radiated loss. The use of high transmission elements helps mitigate this problem.

It is also important to consider that the design of gratings is in many cases specific to the application in which they are used. For instance, if size limitations must be considered then it may beneficial to use elements with high coupling since a higher plasmon output can be achieved over fewer number of elements and thus less physical distance. Some of the high transmission, low coupling elements such as a 140nm wide thin film structure provide high plasmon over a large number of elements showing a peak output at 50-60 elements. These grating structures are more advantageous where size considerations are not an issue.

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