Coupling of energy from quantum emitters to the plasmonic mode of V groove waveguides: A numerical study

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This work is a theoretical investigation into the coupling of a single excited quantum emitter to the plasmon mode of a V groove waveguide. The V groove waveguide consists of a triangular channel milled in gold and the emitter is modelled as a dipole emitter, and could represent a quantum dot, nitrogen vacancy in diamond, or similar. In this work the dependence of coupling efficiency of emitter to plasmon mode is determined for various geometrical parameters of the emitter-waveguide system. Using the finite element method, the effect on coupling efficiency of the emitter position and orientation, groove angle, groove depth and tip radius, is studied in detail. We demonstrate that all parameters, with the exception of groove depth, have a significant impact on the attainable coupling efficiency. Understanding the effect of various geometrical parameters on the coupling between emitters and the plasmonic mode of the waveguide is essential for the design and optimisation of quantum dot – V groove devices.

I. INTRODUCTION

Plasmonics is a fast growing field of research with a wide range of possible applications, many of which rely on the key features of strong field enhancement and subwavelength localisation^{1,2}. One such application, proposed in 2007 by Chang *et al.*, is the use of quantum emitters in conjunction with plasmonic waveguides to create single-photon nano-optical transistors³. The active control over plasmon propagation, which can be achieved by quantum emitter – waveguide systems, has further possible applications in the development of single-photon sources, single-photon switches, and nano-optical amplifiers⁴⁻⁸. A critical aspect of such an emitter-waveguide system is the coupling efficiency, which can be defined as the proportion of energy emitted into the plasmonic mode when the quantum

emitter spontaneously transitions from the excited state to its ground state. Aside from the plasmonic channel, the other paths available during relaxation of the emitter are a nonradiative channel (e.g. resistive heating) and the radiative channel, i.e. decay into bulk radiation^{9,10}. The coupling efficiency, often referred to as the spontaneous emission β factor, is therefore the ratio of the spontaneous emission rate into the plasmonic mode to the sum of the decay rates into all three channels.

Coupling of emitters to plasmons has experimentally been demonstrated for quantum dots (QDs) and J aggregates coated on thin metal films¹¹⁻¹³, QDs in gap plasmon waveguides⁶, and for QDs near metal nanowires^{14,15}. There have also been several theoretical studies that consider single emitters in the vicinity of metal structures. The quantum emitter, which could be a QD, a single atom, a nitrogen vacancy in diamond, or similar¹⁶, is often treated as a point dipole with a dipole moment that oscillates in time. For this approximation to be appropriate, the quantum emitter is restricted to small sizes, as the point dipole model does not accurately predict emission properties of relatively large QDs due to the presence of mesoscopic effects¹⁷.

For certain simple geometries, such as planar stratified media and thin metal nanowires, the decay rates into the various channels can be obtained analytically^{9,16,18}. For other structures where no analytical solution can be found, numerical techniques must be employed. In 2010, Chen *et al.* presented a numerical technique that allows the β factor for plasmonic waveguides with arbitrary cross-sections to be determined¹⁰. Using this technique, the coupling of emitters to a number of different waveguides, namely square, wedge, V groove, and slot, was investigated^{4,10,19-21}. An important consideration in the choice of an emitter-waveguide system is the techniques that are available for fabrication. Unlike chemically synthesised nanowires, nano-scale precision of the waveguide position can be attained during lithographic fabrication. This should enable more precise positioning between the emitter and the waveguide.

The V groove waveguide can be fabricated lithographically and exhibits some further desirable properties, such as low sensitivity to structural imperfections, the possibility to incorporate bends with relatively low losses, and compatibility with planar technology²²⁻²⁴. Detailed analyses of its channel plasmon polariton (CPP) modes can be found in the literature²²⁻²⁶. The coupling efficiency between an emitter and the fundamental plasmonic mode of this waveguide was established to be high

by Martin-Cano *et al.*⁴ and Tudela *et al.*¹⁹ for the case of silver, with efficiencies reaching 90%. In both references, the strong potential of the V groove waveguide for coupling applications has been demonstrated^{4,19}.

Motivated by these findings, it is of interest to gain an in-depth understanding about the coupling between emitters and the fundamental mode of the plasmonic V groove waveguide. Here, we present a detailed investigation into the dependence of coupling efficiency on geometrical parameters of the system using the finite element method (FEM). In particular, we determine the coupling efficiency as a function of vertical emitter position, groove angle, and groove depth. The effect of tip radius, emitter orientation, and horizontal emitter position is also considered. To the best of our knowledge, this is the first time the dependence of coupling efficiency on groove angle, groove depth, tip radius, and horizontal emitter position is presented in the literature. An understanding of the role various geometrical parameters play in coupling applications is imperative for the optimisation and design of QD – V groove devices.

II. METHOD

To study the coupling of QDs to V groove devices, we must first define the waveguide geometry. Figure 1 is a schematic of the waveguide cross-section, illustrating some of the geometrical parameters relevant to this study.

Figure 1: Schematic of waveguide cross-section, illustrating the characteristic parameters: groove depth (d), tip radius (r), and groove angle (θ).

Due to limited resolution, a realistic fabrication process would result in a rounded tip. The radius of curvature is denoted by the tip radius (r). Unless otherwise stated, a tip radius of 2 nm is used within this work. The other V groove parameters are groove angle (θ) and groove depth (d), both of which are allowed to vary throughout the main part of the investigation. For all of the simulations

in this article, a vacuum wavelength of 632.8 nm is used, the dielectric is taken to be vacuum with relative permittivity $\epsilon_{vac} = 1$, and the metal is gold with relative permittivity $\epsilon_{Au} = -9.5 + 1.13i^{27}$. Internal losses of the quantum emitter are fixed to zero.

As indicated in the introduction, coupling efficiency is defined as the rate of spontaneous emission of an emitter into a plasmon ($\hat{\gamma}_{plas}$) divided by the total rate of spontaneous emission ($\hat{\gamma}_{total}$), where both values are normalized with respect to the total decay rate of the emitter in vacuum (γ_0), i.e. in the absence of a metallic structure:

$$\beta = \frac{\hat{\gamma}_{plas}}{\hat{\gamma}_{total}}. \quad (1)$$

The numerical technique used in this work to obtain coupling efficiencies is detailed in Reference 10. The derivation will not be repeated here but for the convenience of the reader, we state the main results, i.e. the equations which contain the quantities of interest. It should first be noted that there are two assumptions underlying the derivation of these main results: 1) Only one guided mode is primarily excited by the emitter and 2) this fundamental plasmonic mode experiences low losses. V groove waveguides are able to support multiple modes, but they can be designed for single-mode operating conditions. This can be achieved by either increasing the groove angle or decreasing the groove depth sufficiently so that all higher order modes are cut off^{24,25}. The range of groove angles and depths used in this investigation, which ensure single mode operation, are 12° to 40° and 120 nm to 180 nm, respectively. The ratio of imaginary part to real part of the propagation constant for the plasmonic mode, which is an indication of losses, ranges from 3% to 8%, depending on groove angle. As detailed in Reference 10, $\hat{\gamma}_{plas}$ can be found as:

$$\hat{\gamma}_{plas}(x, y) = \frac{3\pi c \epsilon_0 |\hat{n} \cdot \mathbf{E}(x, y)|^2}{k_0^2 \int (\mathbf{E} \times \mathbf{H}^*) \cdot \hat{z} dA}, \quad (2)$$

where c is the speed of light, ϵ_0 is the permittivity of free space, $\hat{n}$ is a unit vector parallel to the orientation of the emitter's dipole moment, k_0 is the vacuum wavenumber, $\mathbf{E}$ and $\mathbf{H}$ are the electric

and magnetic fields, respectively, and $\hat{\mathbf{z}}$ is a unit vector along the length of the waveguide. (x, y) denotes the coordinates of the emitter and the integral is evaluated over the entire computational domain transverse to the waveguide, i.e. the x - y plane. In this work we have used a 2D finite element model to determine the fields of the fundamental plasmonic mode. These simulations, as well as the simulations required for later steps, were carried out with the commercial finite element modelling package COMSOL Multiphysics.

From Eq. (1) it is evident that the normalized total spontaneous emission rate is needed for the calculation of coupling efficiencies. The normalized total spontaneous emission rate ($\hat{\gamma}_{total}$) can be determined by 3D simulations with the dipole modelled as a short line current and is given by

$$\hat{\gamma}_{total} = \frac{\int_V \text{Re}(\mathbf{J}^* \cdot \mathbf{E}) dV}{\int_V \text{Re}(\mathbf{J}^* \cdot \mathbf{E}_0) dV}, \quad (3)$$

where $\mathbf{J}$ is the current source, $\mathbf{E}$ is the electric field in the presence of the waveguide, $\mathbf{E}_0$ is the electric field in vacuum, and the integrals are evaluated over the source volume V .

III. RESULTS AND DISCUSSION

The first step in calculating the spontaneous emission factor β is to choose the orientation of the emitter so that one can calculate the plasmonic decay rate, Eq. (2). To determine the orientation which gives the highest plasmon decay rate, the x , y and z components of the CPP mode field profile was calculated. Figure 2 depicts a typical field profile of the fundamental mode in a plasmonic V groove waveguide for the x component of the electric field. The x component of the field is the largest component, and for the majority of this study and unless otherwise indicated, the emitter orientation is taken to be in the x direction.

Figure 2: Field profile of fundamental plasmonic mode for the E_x component.

The position of the maximum field strength is at a small but nonzero distance from the tip, above which point the field strength decreases with increasing height²⁴. From Eq. (2), $\hat{\gamma}_{plas}$ is proportional to $|\mathbf{E}_x|^2$ when the dipole moment of the emitter is parallel to the x axis, so the normalised spontaneous emission into the plasmonic mode is largest wherever the field is strongest. However, this does not necessarily mean that β will be highest at the field maximum. The coupling efficiency, which takes into account all of the decay channels, may actually be low at the position of the field maximum. This is due to the fact that at small distances from the metal, the decay is dominated by the nonradiative contribution²⁸.

Two of the most important pieces of information for the practical realization of emitter – plasmon coupling are 1) the maximum obtainable β factor, and 2) the vertical emitter height at which this efficiency is reached (h_{opt}). These key features of the simulation results are summarised for each setting of groove angle and groove depth in Figure 3.

First of all, from Figure 3 (a) it is evident that the β factors show considerable variations of close to 20% across the graph. These variations are predominantly due to the effect of groove angle. Although groove depth has a smaller effect, there is still some variation in β with changing depth and the variation depends on the setting of groove angle.

To explain these results, it is useful to consider the role various decay channels play and the way they are influenced by groove angle and depth. Let us start by considering groove angle. Emission into the nonradiative channel is strongly dependent on the distance between the emitter and the metal. Small distances lead to quenching (nonradiative decay) being the dominant decay mechanism which competes with the plasmonic decay channel²⁸. Clearly, increasing the groove angle

increases the distance between the emitter and the closest metal surface for a given vertical emitter position. This means that with increasing groove angle, the nonradiative decay rate for the emitter positioned at some vertical height decreases. At the same time, this is accompanied by a change in the plasmonic decay rate due to changes in the field distribution. At very small angles, the field strength of the plasmonic mode is large, but quenching due to the proximity of the metal dominates. At the other extreme, with angles approaching 40° , the field strengths of the plasmonic mode and hence decay rates into plasmons fall off so significantly that the decrease in quenching cannot overcome this effect. Between these limiting cases, there is a region of groove angles which yields large β factors, of 0.8 and upwards, Figure 3(a).

Figure 3: Parametric surface plots summarising key features of simulation results. (a) Maximum coupling efficiency as a function of groove angle and groove depth. (b) Optimal emitter height as a function of groove angle and groove depth.

In Figure 3 (b), a general trend of increased values of the optimal emitter height with increasing groove angle can be observed. This is expected, because as the groove angle is increased the field undergoes a shift, as indicated by the fact that the field maximum moves up the groove and

thus the optimal height for $\hat{\gamma}_{plas}$ increases. Also, as the emitter is moved further up the groove, the nonradiative decay decreases due to larger distances to the metal. A notable feature of Figure 3(b) is the abrupt change in optimal emitter height at small groove depths. The origin of this is clarified in Figure 4, which shows β as a function of emitter height at a groove depth of 120 nm, for the two angles between which the abrupt change occurs at this depth, 26° and 28° .

Figure 4: Coupling efficiency as a function of vertical emitter height, illustrating the origin of the abrupt change in optimal emitter height for $d=120$ nm between $\theta=26^\circ$ and $\theta=28^\circ$.

The curves exhibit two local maxima, with the local minimum of the graph corresponding to the emitter positioned at the top of the groove, i.e. at the same height as the planar dielectric-metal interface. The existence of the two maxima can be explained as follows: if an emitter is within the groove (i.e. for emitter heights below the value of the groove depth) the nonradiative decay is substantial due to the proximity of the metal surface. The nonradiative decay rate decreases with increasing emitter height as a result of increased emitter-metal separation. At the same time, field localisation decreases with increasing emitter height, resulting in a decrease of the plasmonic decay rate. The counterplay between these two effects results in the first maximum. As the emitter height is further increased so that the emitter now lies outside of the groove, the field strength of the plasmonic mode at the emitter position decreases. There is also a rapid change to the nonradiative decay rate, because as the emitter is moved from inside to outside of the groove, the distance to the metal surface quickly increases. Hence, the decay rate into the nonradiative channel drops significantly, and this is the reason for the increase in coupling efficiency when the emitter is at a small distance above the

planar metal surface. When shifting the emitter even higher, eventually the electric field strength of the plasmonic mode becomes so weak that the coupling efficiency falls off. In this regime, it is likely that the decay is dominated by the contribution to the radiative channel. Comparing the curves corresponding to the two groove angles in Figure 4, it is evident that the abrupt change in optimal emitter height from Figure 3 (b) can be attributed to the transition of the global maximum from the first local maximum at the lower angle to the second local maximum at the higher angle.

To further investigate the dependence of the β factor on vertical emitter positioning, Figure 5 contains plots of β as a function of emitter height for various groove angles. There is a considerable change in the dependence of β on emitter height for the various groove angles displayed in Figure 5. Aside from the fact that the global maximum shifts towards larger emitter heights with increasing groove angle, the shape of the curves also changes with increasing angle; flattening out as the angle is increased. This flattening of the curves is related to the sensitivity of β to the emitter height: at small angles the range of emitter heights which give similar β factors to the maximum value is small, but this range increases with increased groove angle. Due to challenges in positioning quantum emitters with nano-scale accuracy, the sensitivity of coupling efficiency to the emitter height may be an important consideration for practical applications. Even though larger angles can give smaller β values, the sensitivity of β to emitter height can be reduced.

Figure 5: Coupling efficiency as a function of vertical emitter height, for different groove angles, $d=120$ nm.

At low angles, the optimal emitter position is within the groove while at large angles the optimal emitter position is above the groove, Figure 5.

Further simulations were performed to explore the dependence of the coupling efficiency on emitter orientation, tip radius, and horizontal emitter position. These were compared to a reference simulation at $\theta = 26^\circ$, $d = 150$ nm, $r = 2$ nm, with the emitter's dipole moment parallel to the x axis. A change of the emitter's dipole moment to be parallel to the other axes resulted in negligible coupling efficiencies for the emitter positioned above the centre of the groove. Results for varied tip radii are depicted in Figure 6. It can be noted that there is a moderate effect of tip radius for the setting of 26° .

Figure 6: (a) Normalised decay rate into plasmonic mode ($\hat{\gamma}_{plas}$) as a function of vertical emitter height, for different tip radii. (b) Coupling efficiency as a function of vertical emitter height, for different tip radii. Both at $\theta=26^\circ$, $d=150$ nm.

From Figure 6 (a) it is evident that when the tip radius is increased, the normalised spontaneous emission into the plasmonic mode is significantly reduced at low emitter heights. This is expected, because as the tip radius is increased, the field of the fundamental plasmon mode becomes more delocalised and there is less field strength at the emitter positioned at low emitter heights²⁴. If the radius of curvature is allowed to continue increasing, eventually a point will be reached at which

the CPP mode ceases to exist, leaking out of the groove and turning into a surface plasmon²⁴. At large emitter heights the $\hat{\gamma}_{plas}$ values are small, but for larger tip radii the values slightly exceed those of the lower radii, as the maximum of the plasmonic mode moves up the groove with increasing tip radius²⁴.

In Figure 6 (b), it can be observed that the attainable β factors are slightly higher for increased tip radii and are found at large emitter heights for these radii. Though this may seem contradictory at first glance, the physical reason behind this behaviour may be that the nonradiative decay decreases as the emitter height is increased, and the plasmonic decay is higher at large emitter heights for large tip radii, Figure 6 (a).

The final geometrical parameter considered in this study is horizontal emitter position. Fig. 7 illustrates the sensitivity of coupling efficiencies to the horizontal emitter position, for a number of different emitter heights within the groove. Within 10 nm on either side of the central position the β factor is fairly robust, while a larger deviation leads to a significant drop in coupling efficiency. This can be attributed to the proximity to a metal surface, which also explains why the drop is more pronounced for lower emitter heights, i.e. where the emitter is closer to the metal and the nonradiative decay tends to dominate.

Figure 7: Coupling efficiency as a function of horizontal emitter position, for different emitter heights ($\theta=26^\circ$, $d=150$ nm, $x=0$ nm corresponds to centre of the groove).

IV. CONCLUSION

In summary, the effect of changing geometrical parameters of the emitter - V groove system on coupling efficiency has been investigated using FEM simulations. From the simulation results it was found that the groove angle plays a substantial role in the maximum obtainable coupling efficiencies; there is a range of intermediate angles which result in maximal β factors. In contrast, groove depth plays a less defining role, despite a small interactive effect together with groove angle. However, both groove angle and depth affect the optimal position of the emitter, which is an important aspect in the design of QD – V groove devices.

The emitter orientation is crucial since, at least for emitters centrally positioned above the groove tip, only emitters oriented along the x direction yield good coupling efficiencies, while the other orientations give efficiencies close to zero. The efficiencies are not very sensitive to horizontal emitter positioning within a small region around the centre, but fall off significantly when approaching the metal. The tip radius of the V groove was also found to have a significant impact on both the maximum coupling efficiency and the optimal emitter height, with large tip radii actually yielding higher β factors.

Due to the demonstrated sensitivity of the emitter – plasmon coupling to many of the geometrical parameters of the system and the presence of interactive effects, detailed knowledge about the parameter settings is required to accurately predict the coupling. Conversely, when certain parameters such as tip radius and limited precision of the QD positioning are dictated by practical circumstances, the other parameter settings could be adjusted to optimise the coupling efficiency. Therefore, the geometrical parameters are expected to play an important role in the design of QD – V groove devices.

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