Validation Report

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Modelling Plasmon Mode Prapagation in OmniSim

Abstract

The purpose of this report is to illustrate a way to model plasmon mode propagation using OmniSim, calculating the effective index and loss of the plasmon modes. Also, we will compare the results from OmniSim (using the numerical FDTD algorithm) with the results obtained by the semi-analytical FMM (Film Mode Matching) and effective index methods of Fimmwave.

Modelling guidelines

In order to model the propagation of a plasmon, we first have to excite it. The way to do that is e.g. as shown on Fig. 1. The basic idea is that some of the light created by the Gaussian or dipole excitors will couple to the plasmon mode, and will propagate along the metal-dielectric interface. The rest will radiate away. The easiest way to measure the loss is to put two sensors near the dielectric-metal interface. We can calculate the flux of both sensors. Then the loss of the mode will be

$$a = -\frac{\ln(T)}{D} \qquad (1)$$

where $T = \frac{F_{output}}{F_{reference}}$ (2) is the ratio of the positive flux of the output (second) sensor over the positive flux of the reference (first) sensor. D is the distance between the two sensors. α expresses the rate at which the power in the plasmon decrease with distance :

$$P = P_o \cdot e^{-az} \qquad (3)$$

and has units of 1/length. Another other useful parameter is the propagation length, defined as the length at which the power falls to 1/e of the original power, and is equal to

$$L_p = \frac{1}{a} \qquad (4)$$

where L_p is the propagation length and α is the loss

The propagation constant β can be measured in a similar way, by measuring the phase at the two sensors:

$$\beta = \frac{\phi_{output} - \phi_{reference}}{D} \qquad (5)$$

where D is again the distance over the two sensors.

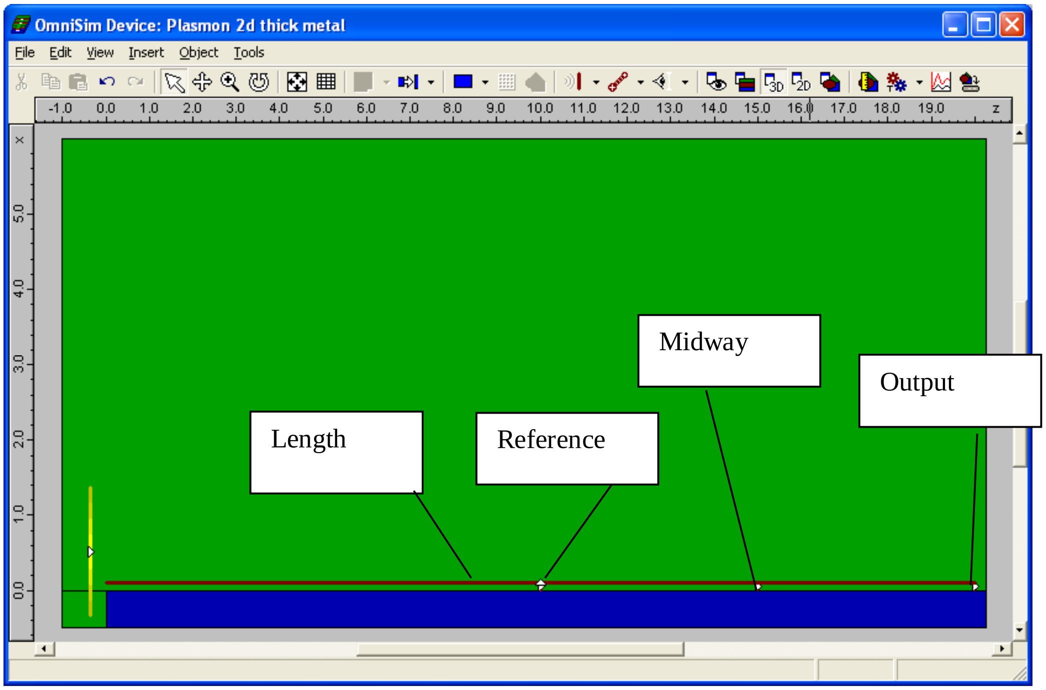

Figure 1: Setup to measure the plasmon propagation loss. The excitation is performed by a Gaussian excitor. We see the three little sensors, labelled as Reference, Midway and Output, and the Length Sensor (the long sensor parallel to the metal). Green is a dielectric of refractive index of 1.595 and blue is gold. The wavelength of interest is 1.55um.

The parameters one has to control in order to have an accurate measurement, are the following:

1) **Number of excited modes**: There might be more than one mode excited. These will probably be radiation modes and attenuate quickly, but we have to ensure that they are of negligible amplitude between the sensors where we perform the measurement. There are two ways to check that. One is to put a third sensor between Output and Reference, called Midway. If the loss we calculate between Output/Reference, Midway/Reference and Output/Midway is the same, then we can be sure that we have only one mode.

Another way to check that is to put a long sensor along the propagation direction, and plot the field vs position from it. If there is one mode travelling, we should se an exponential attenuation, or a straight line in a log plot. We can also measure the loss from the data of the Length sensor. If we are plotting field amplitude, and H_1 and H_2 are the values of the field at two points with distance D between them, then the loss is:

$$a = 2\frac{\ln\left(H_2 / H_1\right)}{D} \qquad (6)$$

2) **Grid size**: We have to ensure that the grid size we are using is fine enough to describe the propagation of light in the metal. One rule of thumb is to choose a grid equal to or smaller than the skin

depth. The skin depth is defined as the distance in the metal where the power falls to 1/e of the original and is equal to

$$\delta = 1/a_{material} \qquad (7),$$

where δ is the skin depth and $\alpha_{material}$ is the material loss of the metal. If the complex refractive index of the metal is $N=n+i\kappa$, then

$$n^2 - \kappa^2 = \varepsilon_r \qquad (8a)$$

$$2n\kappa = \frac{\mu\sigma}{\omega\varepsilon_o} \qquad (8b)$$

where ε_r is the relative dielectric constant of the metal, μ is the magnetic permeability, σ is the conductivity of the metal and ω the angular frequency of the field. ε_o is the dielectric constant in vacuum. Then we have

$$\alpha_{material} = \frac{4\pi}{\lambda}\kappa .$$

For a metal we are usually able to ignore n in (8a) as much smaller that κ, and calculate κ directly from there.

3)**Simulation size**: Here we simply have to ensure that the plasmon mode is practically zero at the boundaries of the simulation. If the mode has a significant amplitude at the absorbing boundaries, it might be extra attenuated, and we will get an incorrect measurement.

Grid Size

The first thing we had to do is to establish the required grid size to accurately model the propagation of light in the metal. What we expect from theory, is that the grid should be fine enough to sample the spatial frequency with which the field varies in the metal, in other words, the grid must be smaller than the skin depth. The skin depth can calculated by Eq. (7) . For gold at 1.55 um we get a skin depth of about 12nm. Therefore we should get good results with a grid of 12.5nm, but for more accuracy we might need to go to 6.25nm.
We modelled the structure of Fig. 3. The reason we chose this structure is that it minimises the effect of the boundary conditions, since light decays in the metal before reaching the boundaries. (Getting PML boundaries right in FIMMWAVE is an additional complication we wish to avoid here.)

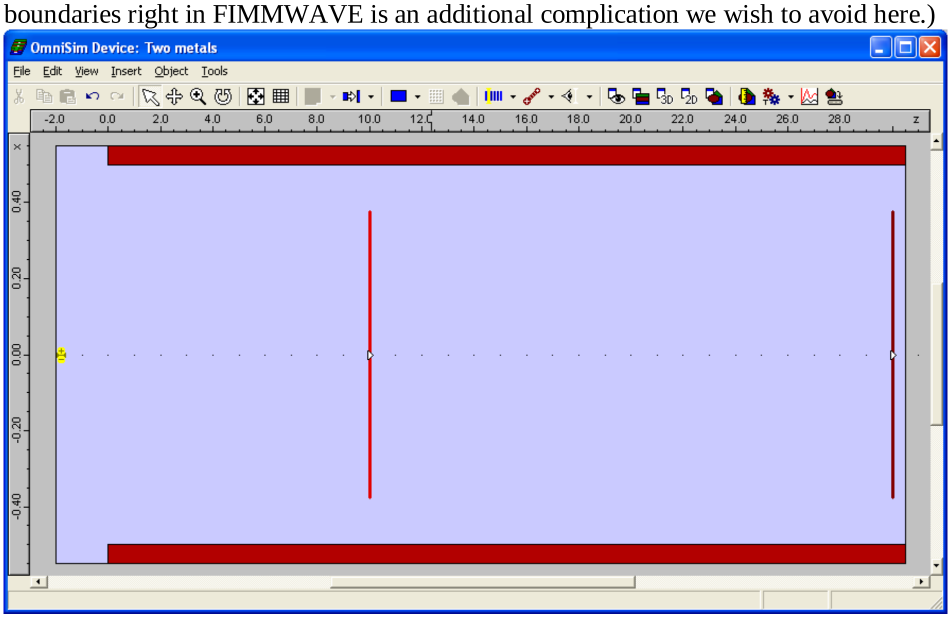

Figure 2: Simulated structure for investigating the effect of the grid size. The air gap was 1um. Negative and positive x-direction boundaries are electric walls.

We ran several simulations, with various widths of the metal layers. The results can be seen in Table 2. We also tried the subgridding feature in the metal layers

Metal Thickness (um)	Loss (1/cm)					
	Fimmwave	OmniSim (grid size below, in um)				
		0.025	0.0125	0.00625	0.025 with 4x subgrid	0.025 with 8x subgrid
0.025	45.34	3.86	19.53	33.2		
0.05	108.829	71.3	94	101.91	92	91.78
0.1	131.0377	122.56	126.415	127.12		
0.5	131.7799	125	129.32			

Table 1: Simulation results for various grid sizes and thickness of the metal layer.

As we see from the table, the loss converges with the thickness of the metal, as expected. The thinner the metal layer, the thinner the grid required to give an accurate result. The result from Fimmwave is very accurate, as it is a 1D structure. For 1D structures the effective index solver we used is extremely accurate since it is a semi-analytical method.
For a layer of 0.05um, we see that a grid size of 0.00625um yields accurate results (within 10%). For thicker metal layers, a coarser grids yield good results. The subgridding increases the accuracy of the major grid (66% to 85% for major grid of 0.025um), but is still less accurate that a major grid of the same size as the subgridding. However, it seems that we can be accurate within 20% with the subgridding.

Simulation size

The easiest way to determine the required simulation size is to have an idea of the extent of the mode already, e.g., if you have a mode solver. We used Fimmwave to find the plasmon mode for the cross section of Fig. 1. The plot can be seen on Fig. 3. We see that after 6um from the metal dielectric interface, the mode has practically attenuated to zero.

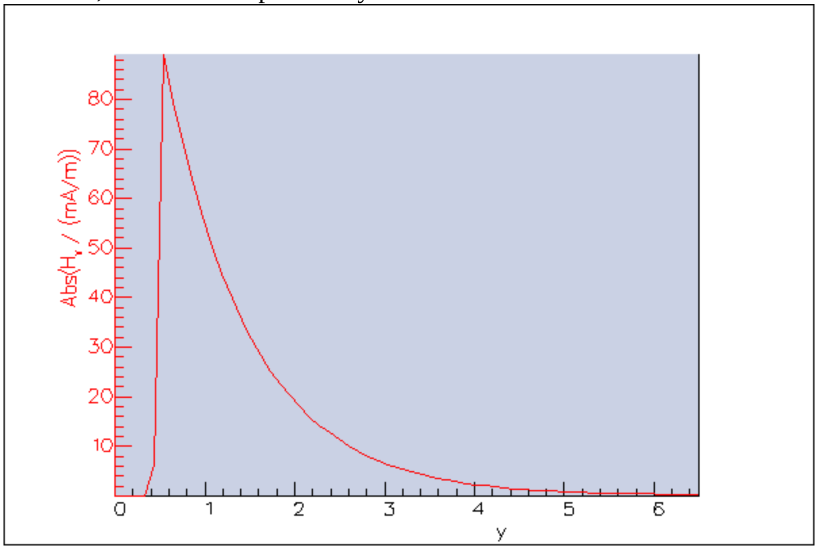

Figure 3: plasmon mode from Fimmwave. We see that the field has completely decayed at 6um from the metal-dieletcric interface, which is located at 0.5um.

If however we do not have a mode solver, we have to estimate the size of the simulation area. Some trial and error will be inevitable; we will have to increase the size and measure the loss, until we see it converging somewhere. We can have a rough idea if the width is large enough, if we put a sensor along the x-direction as shown in Fig. 4. The field plots versus x for two cases, one of large and one of small width can be seen on Fig. 5. It is advisable to put the Transverse profile sensor at a fairly large distance from the excitation, so that all higher order modes have radiated away.

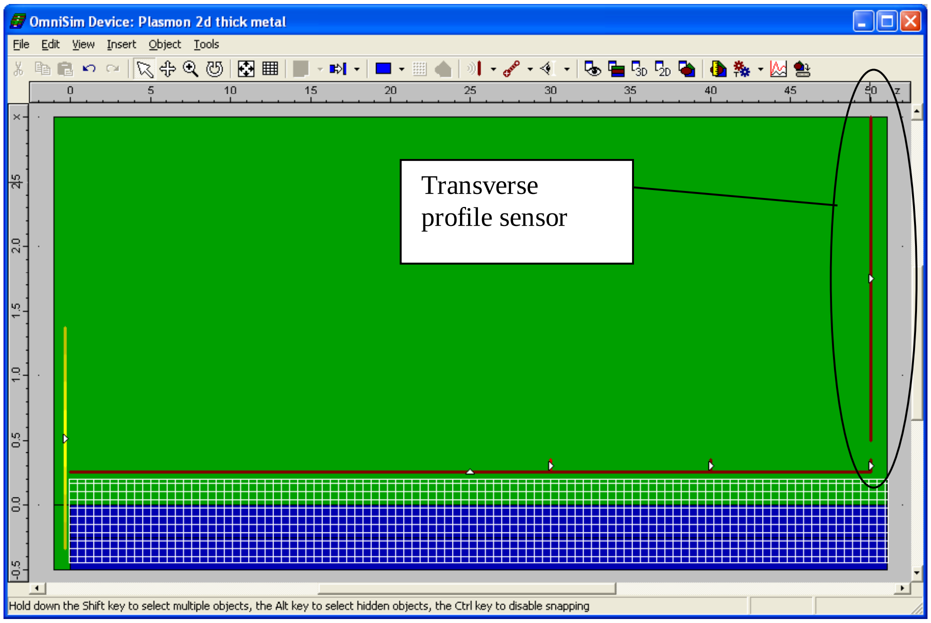

Figure 4: Coarse grid (50nm) test to compare the case where the width is adequate and the width is small.

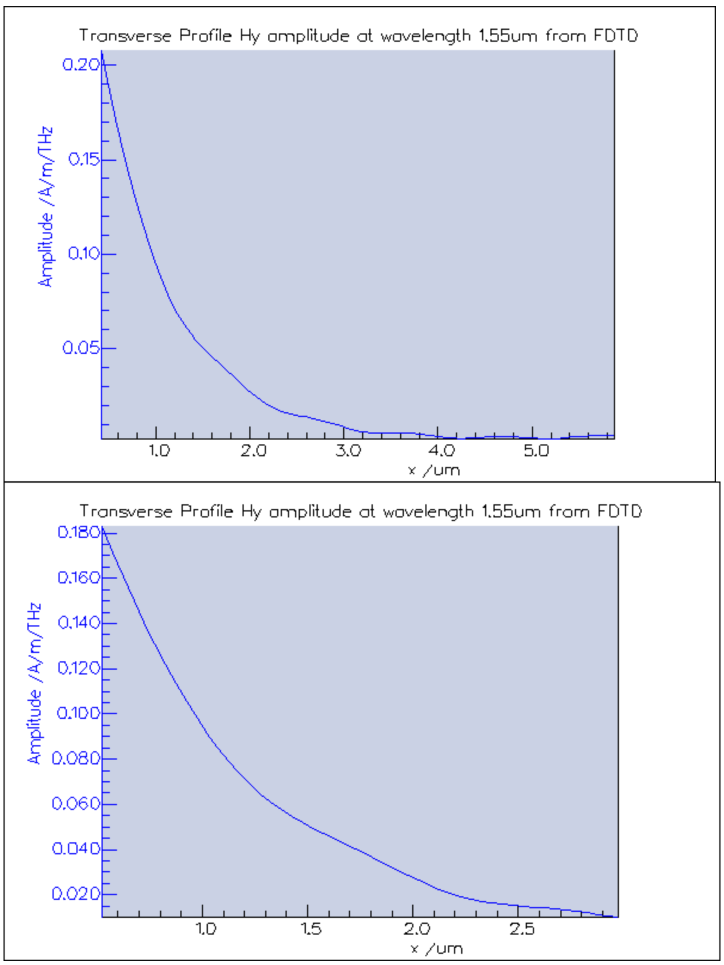

Figure 5: Magnetic field plot for an adequate width (top – 6um) and a small width (bottom – 3 um).

2D simulation

We do a 2D simulation of the structure in Fig. 1. The z-position of the reference sensor was at 10um, Midway was at 20um and Output was at 30um. The modified structure (different length) can be see in Fig. 6.

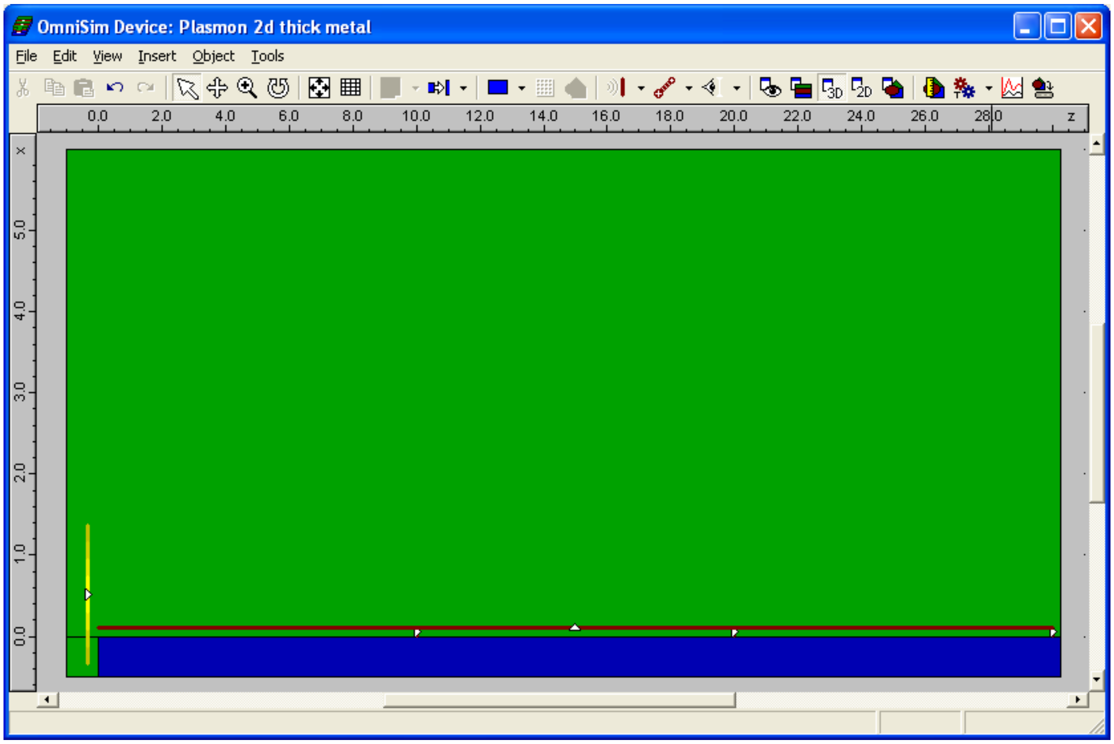

Figure 6: Structure for a 2D simulation.

The results we obtained are seen in Table2. We calculated them by applying Eq. (1) and (6). We see that we get a higher loss from Midway/Reference than from Output/Midway. This is probably because of the presence of other modes that have not completely attenuated yet.

	Relative Transmission	Loss(1/cm)	Propagation length	Accuracy (%)
Output/Reference	0.5954	259.2609152	38.57118221	29.20073595
Midway/Reference	0.7595	275.0949569	36.35108441	37.0915121
Output/Midway	0.784	243.3462586	41.09370761	21.26978601
From Length Sensor		262.1047468	38.15268561	30.61793812

Table 2: Loss results for a grid of 12.5nm, and the structure of Fig 3.

We see that we don't get very accurate results, and this should be attributed to the grid size. It is worthy to plot the field amplitude vs z (Fig. 7) and phase vs z (Fig. 8). On Fig 7 we can see the change in the gradient, which shows that in the beginning we have more than one mode propagating, and after about 15um, only the fundamental plasmon mode seems to have significant amplitude, so we see a straight line in a log plot (exponential attenuation).

The most accurate result from Table 2 is from Output/Midway, and should be attributed to higher order modes, which have not attenuate between midway and reference, but are smaller between Output/Midway. Obviously the longer we make our structure the smaller the effect of these higher order modes will be, on the expense of memory and calculation time.

The result calculated from the Length sensor seems to be less accurate and this can be attributed to the following reasons:

1)The Output/Midway/Reference sensors measure positive flux, which shields us from small reflections at the PMLs at the right hand side

2)The Output/Midway/Reference sensors measure the flux through their whole size, while the Length sensor's thickness is just on grid cell.

From the phase plot (Fig. 8) we can calculate the effective index of the plasmon. We measure the phase at 24.9937um and 29.9937um. The easiest way to do that is by exporting the data of the graph to a text file. We have to count the number of whole periods between the two coordinated from the graph. Then we can apply Eq. (5) to get an effective index of 1.638299436, while Fimmwave returns 1.616154413, an accuracy of 1.370229%.

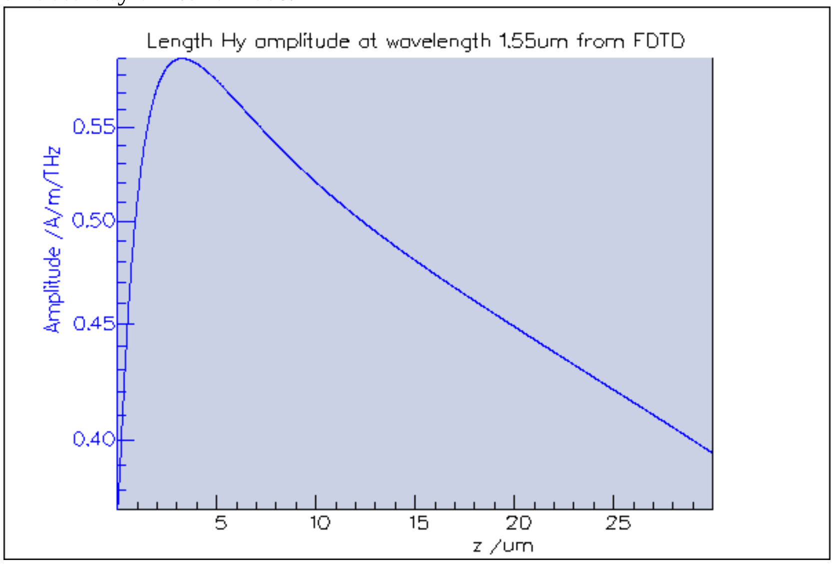

Figure 7: Field amplitude vs z, from the length sensor. Log scale for the y-axis. We see that the field rises in the beginning, as the Gaussian excitation couples to the plasmon mode. Then we see it attenuating. Note the change in gradient, indicating that the radiation modes have almost completely attenuated at about 15um.

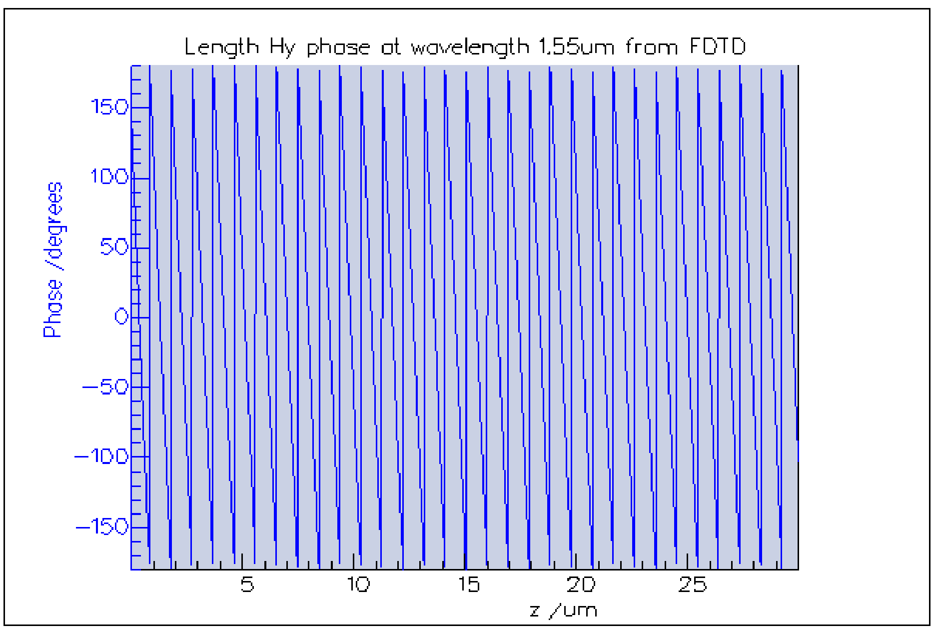

Figure 8: Phase vs z.

We repeat the simulation with a finer grid of 6.25nm, and with a grid of 25nm with a 4x subgridding around the metal-dielectric interface. The 4x subgrid means that the grid size near the metal-dielectric interface will be 6.25nm. The results can be seen on Table 3. We note that the subgridding results are very accurate and require about 10 times less memory and time than simulating the whole structure with the fine grid of 6.25nm. The effect of speeding up the calculation with subgridding is even more evident in 3D calculations.

		Loss(1/cm)	Propagation length	Accuracy (%)
30um long	Output/Reference	222.2069291	45.00309707	10.73515942
6.25nm gird	Midway/Reference	244.7503051	40.85796746	21.96948204
	Output/Midway	199.6711951	50.08233658	**0.495354885**
	Length Sensor	215.197033	46.46904216	**7.241830177**
30um long	Output/Reference	227.6954584	43.91831119	13.47032691
25nm grid + 4x subgridding	Midway/Reference	249.7442331	40.04096461	24.45816869
	Output/Midway	205.794913	48.59206603	**2.556354056**

Table 3: Loss results for the cases of 6.25nm grid and 25nm with 4x subgridding. We see that we get very good accuracies, up tp 0.5% with the 6.25nm grid and 2.5% with the subgrid.

We present two screenshots of plasmon propagation from the simulation with 25nmgrid+4xsubgridding (Fig. 6 and 7).

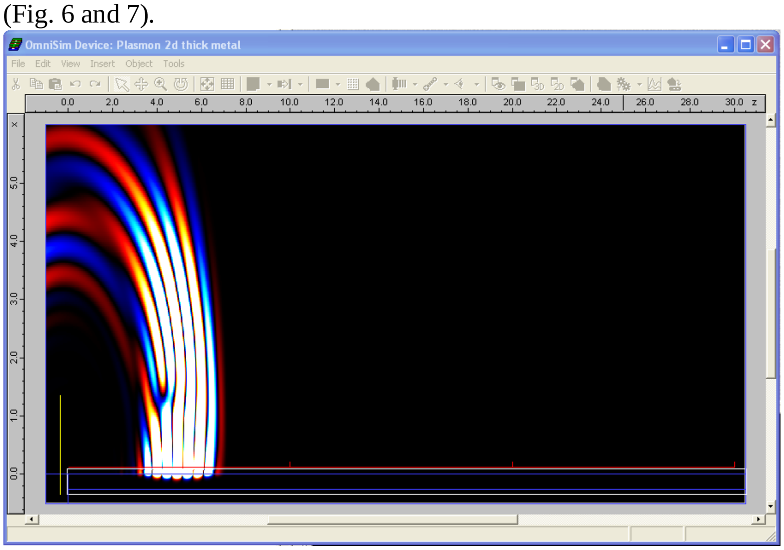

Figure 9: Screenshot of the 2D plasmon mode (Hy plotted). Simulation with 25nm grid+4x subgridding around the metal dielectric interface. We can see that a part of the pulse has coupled to the plasmon mode, while the upper part is radiating away.

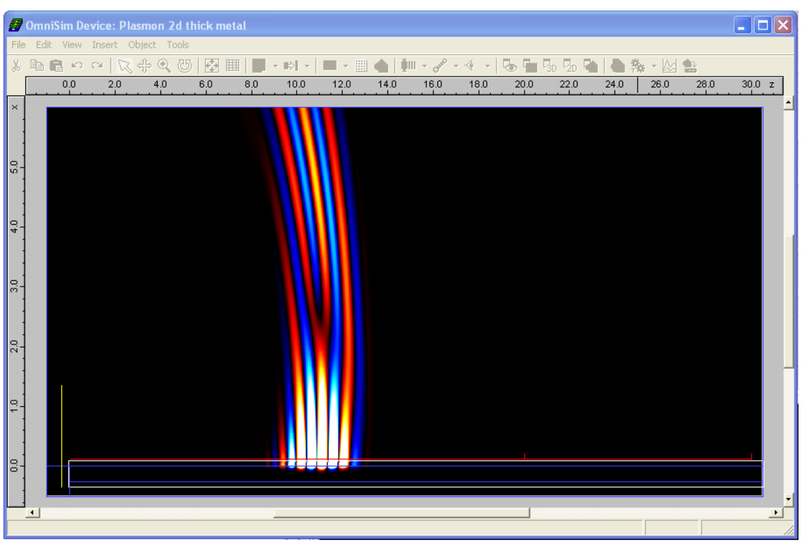

Figure 10: A screenshot of the same simulation as in Fig. 6, but at a later time (Hy plotted). There is still some field radiating away, but near the metal we have the profile we would expect from a surface plasmon.

Finally, in Table 4 we present a different set of simulations we did for the same problem. The differences are a slightly different fit for gold and different locations of the sensors, mainly at different z positions. The main conclusions about the grid size, more than one modes propagating and simulation size are the same.

		Loss(1/cm)	Propagation length (um)	Accuracy (%)
20um long 12.5nm grid	Output/Reference	289.0162955	34.60012517	44.02910692
	Midway/Reference	314.2435115	31.82245498	56.60090117
	Output/Midway	264.3218072	37.83267111	31.72279359
40um long 12.5nm grid	Output/Reference	248.2148717	40.28767467	23.6960229
	Midway/Reference	245.1335692	40.79408639	22.16047885
	Output/Midway	251.4272918	39.7729297	25.29690838
20um long 6.25nm grid	Output/Reference	243.6013932	41.05066834	21.39693042
	Midway/Reference	274.3904784	36.4444133	36.74044047
	Output/Midway	212.944489	46.96059544	6.119291746
30um long 6.25um grid	Output/Reference	199.6589852	50.08539931	**0.501439616**
	Midway/Reference	198.5360033	50.36869803	**1.061069225**
	Output/Midway	201.1882305	49.70469682	**0.260648319**
30um long 25nm grid+ 4x subgridding	Output/Reference	252.572362	39.59261386	25.86754555
	Midway/Reference	280.4791128	35.65327877	39.77466588
	Output/Midway	224.5241087	44.53864691	**11.88990852**

Table 4: Results for the Plasmon loss from OmniSim and comparison with Fimmwave, for various grid sizes and simulation lengths. The numbers in red illustrate the difference in attenuation measure between Output/Midway and Midway /Reference, due to more than one modes propagating. Numbers in bold show the most interesting results, very accurate with an 6.25nm grid, and good, with much smaller time and memory demands, with the subgridding.

3D Simulation

For the 3D simulation the same guidelines as the 2D apply. However, as 3D simulations are lengthy, the user is advised to first do the simulation in 2D, especially the parts that may require trial and error. Once you are reasonably confident that you understand how the structure works and that you have identified the right parameters, then you should move to the 3D simulation.
For the purposes of this validation report we do the following experiment. We identify the plasmon mode of a structure in Fimmwave and then launch this mode into OmniSim, using a mode excitor. The fact that we are launching a Fimmwave mode should minimise the undesired effects, such as higher order mode excitation. However, as OmniSim (FDTD) is a numerical method time-domain method with a finite frequency resolution, the mode generated in Fimmwave, which is a semi-analytical frequency domain method, will be a bit different.
The simulated structure can be seen on Fig. 11. The results can be seen in Table 5.

	Loss(1/cm)	Propagation Length(um)	Accuracy (%)
Output/Reference	308.2975	32.43620204	8.322642884
Midway/Reference	292.4231564	34.19701819	14.20299408
Output/Midway	324.3356789	30.8322539	2.966161842
Pre-Output/Reference	302.760533	33.02940414	10.30367687

Table 5: Results from the 3D simulation of a plasmon mode. Fimmwave loss is 333.956/cm. We see a very good accuracy is attained between Output/Midway.

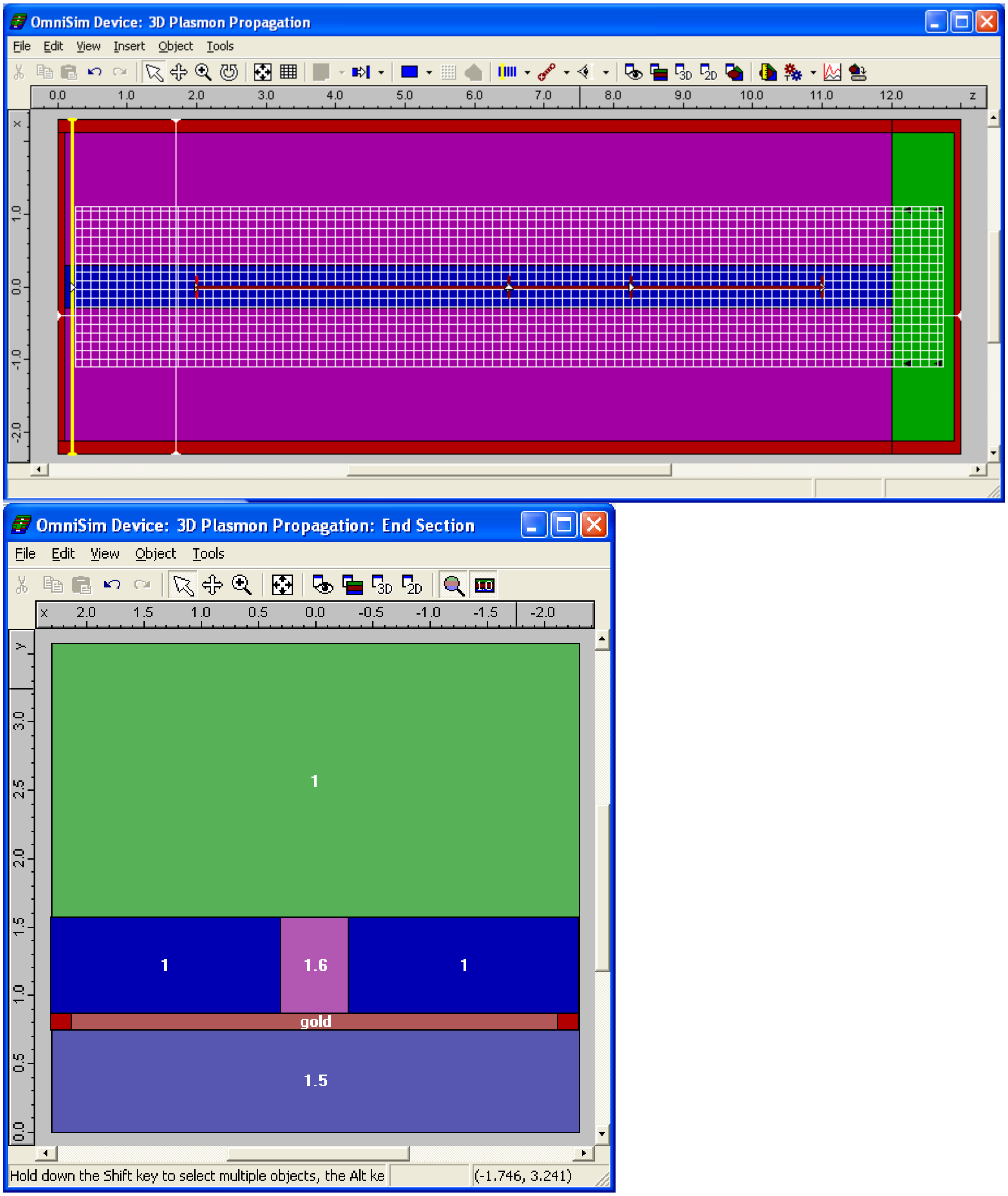

Figure 11: x-z (top) and cross sectional view of the structure. We used a major grid of 25nm with a 4x subgriding in and around the metal.

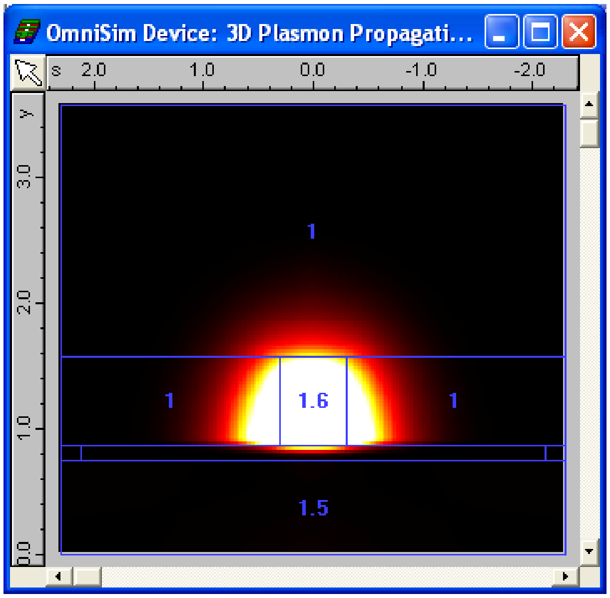

Figure 12: Excitation profile. This is the plasmon mode, generated by Fimmwave, and imported to OmniSim.

From the results at Table 5, it might seem strange that we get a lower loss between Midway/Reference than from Output/Midway. The reason can be seen on Fig. 13, where we see the longitudianal profile of the magnetic field amplitude, along the direction of propagation. We would expect an exponential decay, instead we see something that looks like beats arising from interference between two modes. Note that the size of the beats is much smaller than the size of the average amplitude, therefore this should note influence the result significantly.

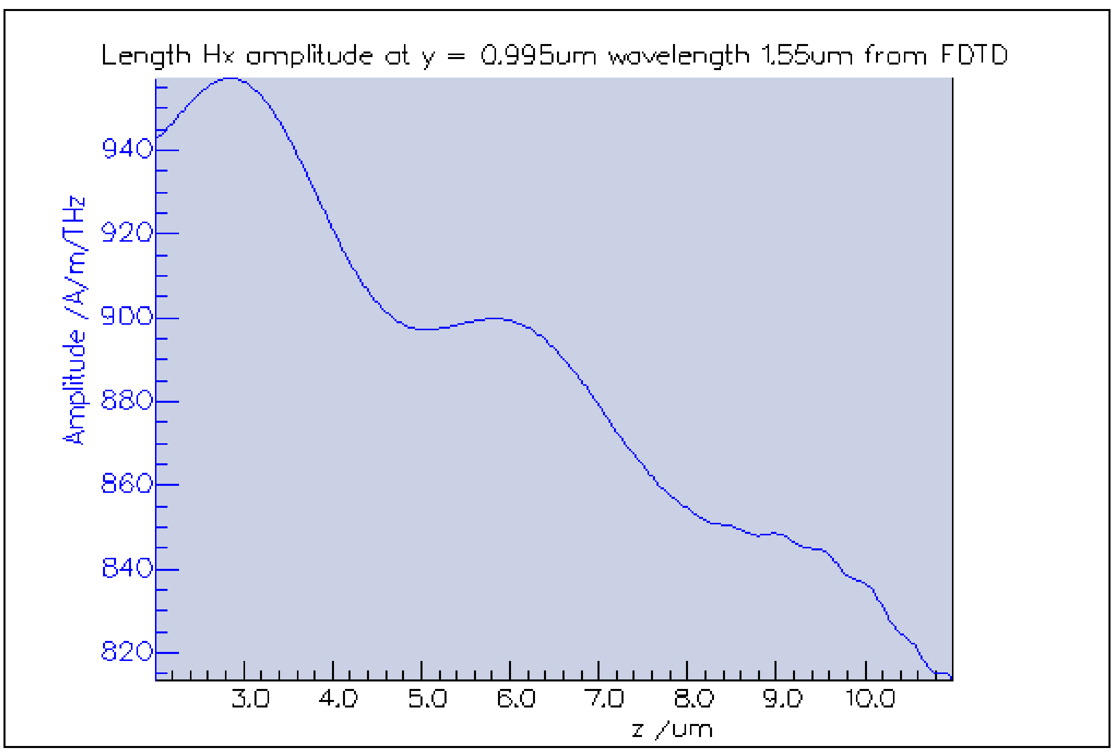

Figure 13: Amplitude of the magnetic field vs z, along the direction of propagation. Instead of seeing an exponentially attenuating ampltude, as we would expect if we had only one plasmon mode, we see something that looks like interference of a strong mode (our plasmon) with a weaker one. Note the scale of the y-axis: these beats are about 2-3% of the main amplitude, therefore they have a minor effect to the result.