Validation Report

Name of Report	The reflection from a thin metal film – a comparison between OmniSim and FIMMWAVE
Performance Date	21st July 2005
Performed By	Stephen Day
Product Name	OmniSim
Product Version & Compile Date	OmniSim v3.1 July 14 th 2005 FIMMWAVE v4.4 July 11 th 2005
References	

The reflection from a thin metal film – a comparison between OmniSim and FIMMWAVE

1. Report Summary

a) The aim of this study was to compare the reflectivity obtained from OmniSim using FDTD and that obtained with FIMMWAVE using eigenmode expansion.

b) To test the material fitting database of OmniSim

1.1. Summary

The validation tests have been performed on a simple mirror and also on a Fabry Perot etalon

Test 1	Absorbing layer with fixed real refractive index and fixed absorption	N= 0.25713363 α= 855251.82	
Test 2	Gold mirror using material database		
Test 3	Tungsten mirror using material database		
Test 4	Aluminium mirror using material database		
Test 5	Nickel mirror using material databse		
Test 6	Resonator using gold mirrors		

1.2. Validation Tests Results

1.2.1. Test 1

The structure considered in this case was a medium of refractive index 1.45 coated with a thin layer of a metallic material, followed by air.
The device is shown schematically in figure 1.

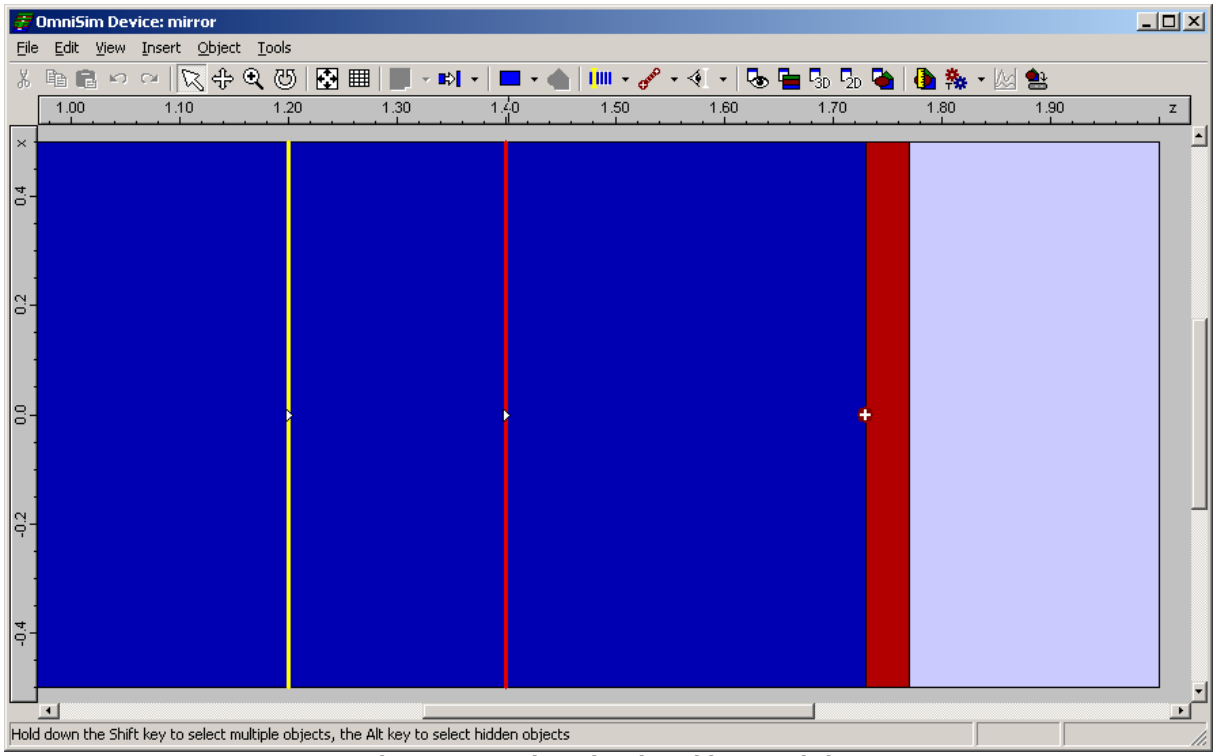

Figure 1: Device simulated in OmniSim

The refractive index of the metallic layer was set to be 0.25713363, with an alpha of 855251.82, these values are representative of gold in the infra red.

In OmniSim a plane wave excitor was used with TE polarisation and electric side walls. A step size of 2 nm was used and 8192 time steps. A PML thickness of 64 grid points was used for all of the FDTD calculations. When one defines an explicit complex refractive index, OmniSim will try to fit a Drude model to the complex refractive index at the excitor wavelength but the fit will be incorrect at other wavelengths. Hence in order to get comparison between FIMMWAVE and OmniSim, it is necessary to run an OmniSim FDTD simulation at each required wavelength and obtain the calculated flux.

In FIMMWAVE, waveguides of constant refractive index were created and the effective index solver was used.

Figure 2 shows the comparison between FIMMWAVE and OmniSim over the wavelength range 1 um to 1.8 um for a 20 nm thick film.

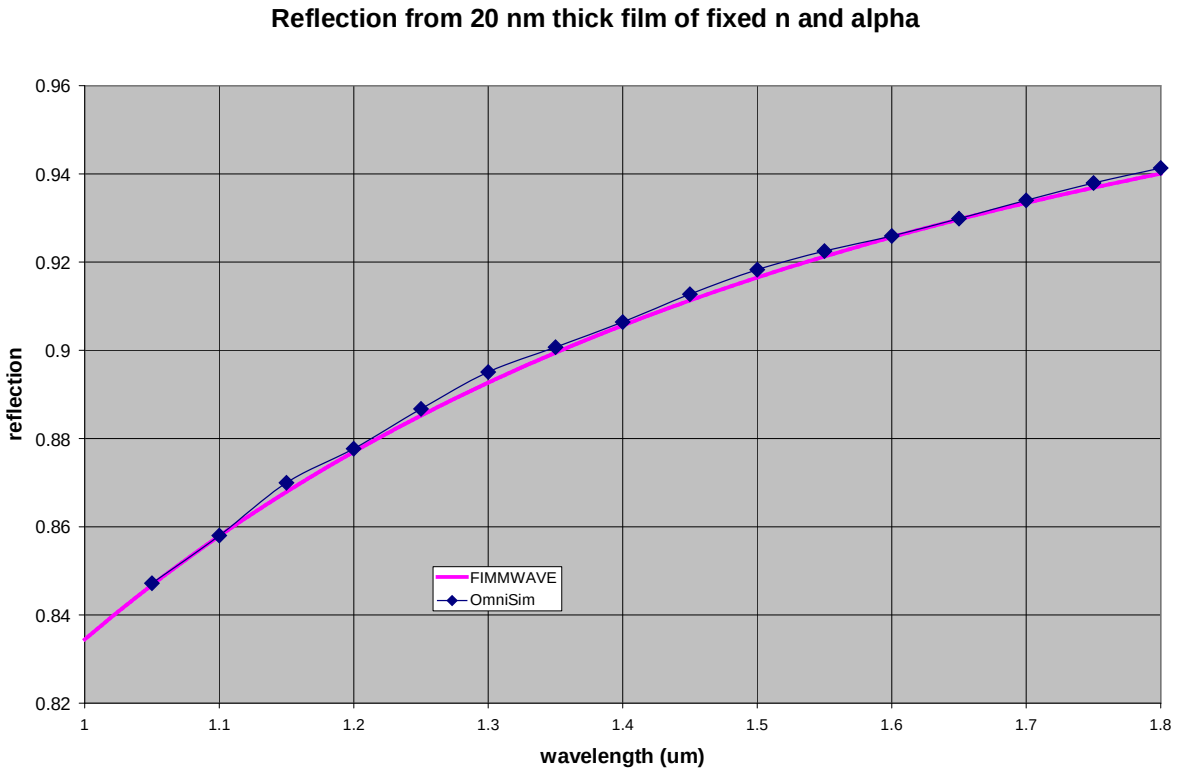

Figure 2: Comparison between OmniSim and FIMMWAVE against wavelength

The agreement over the entire wavelength range is good although the OmniSim results show a slight wavelength dependent ripple. This was determined to be due to reflections from the boundaries and can be significantly reduced by increasing the thickness of the FDTD PML. The maximum difference between OmniSim and FIMMWAVE occurs at 1.5 um wavelength and corresponds to a an error of 0.19%. Figure 2 shows the percentage error between FIMMWAVE and OmniSim as the PML thickness is increased.

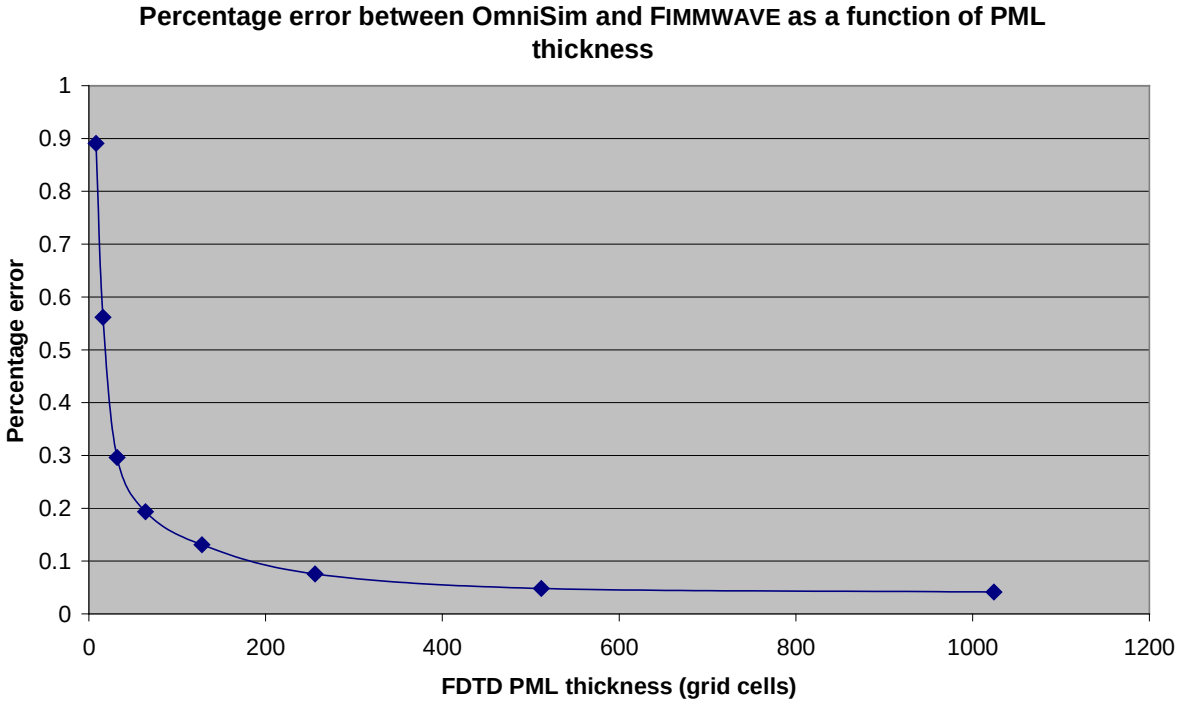

Figure 3: Percentage error between OmniSim and FIMMWAVE

The results show quite clearly that the error comes from reflections and that with a sufficiently thick PML, then the error can be reduced to less than 0.05%. Future versions of OmniSim will have improved PML's to further reduce this error and to avoid the requirement for excessively thick PML's.

The thickness of the film has also been increased from 0 to 40 nm and the results at a wavelength of 1.2 um are shown in figure 4.

Reflection from metallic film at 1.2 um wavelength against film thickness

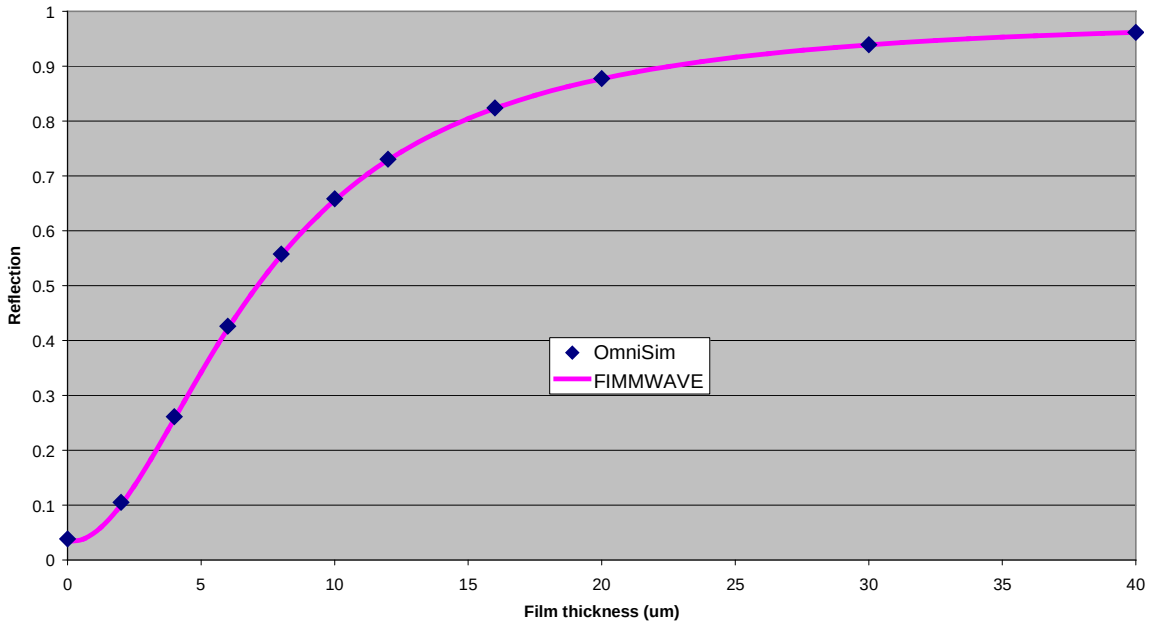

Figure 4: Comparison between OmniSim and FIMMWAVE against film thickness

1.2.2. Test 2

In this test the material database was used to define the refractive index and alpha of the absorbing layer. In FIMMWAVE the material database is used to give the correct value of refractive index and alpha at each wavelength. However in OmniSim a model is used to fit the material data. The models are Drude, Debye and Lorentzian. The accuracy will depend upon the quality of the fit. The fit can be sit automatically by OmniSim or the user can select the model and the wavelength fitting range. To look at the fitted model open the FDTD calculator dialog and then click on the material text box. The FDTD materials parameters dialog box will then open and the fitted models can be plotted. For gold the fit in figure 5 is shown over the wavelength range 1.4 um to 1.8 um.

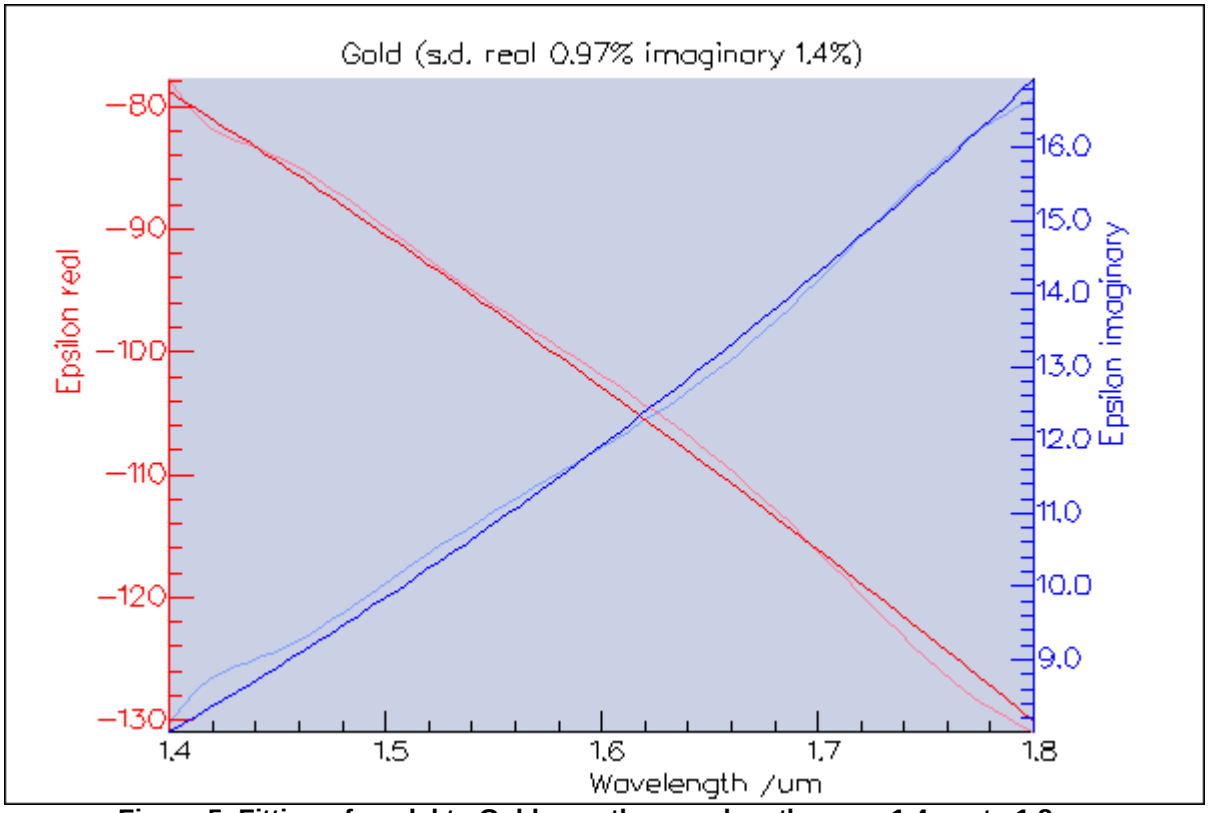

Figure 5: Fitting of model to Gold over the wavelength range 1.4 um to 1.8 um

The fit is accurate to 0.97% in the real index and 1.4% in the imaginary refractive index. If the fit is now extended to cover the wavelength range 1 um to 1.8 um, then the fit shown in figure 6 is obtained.

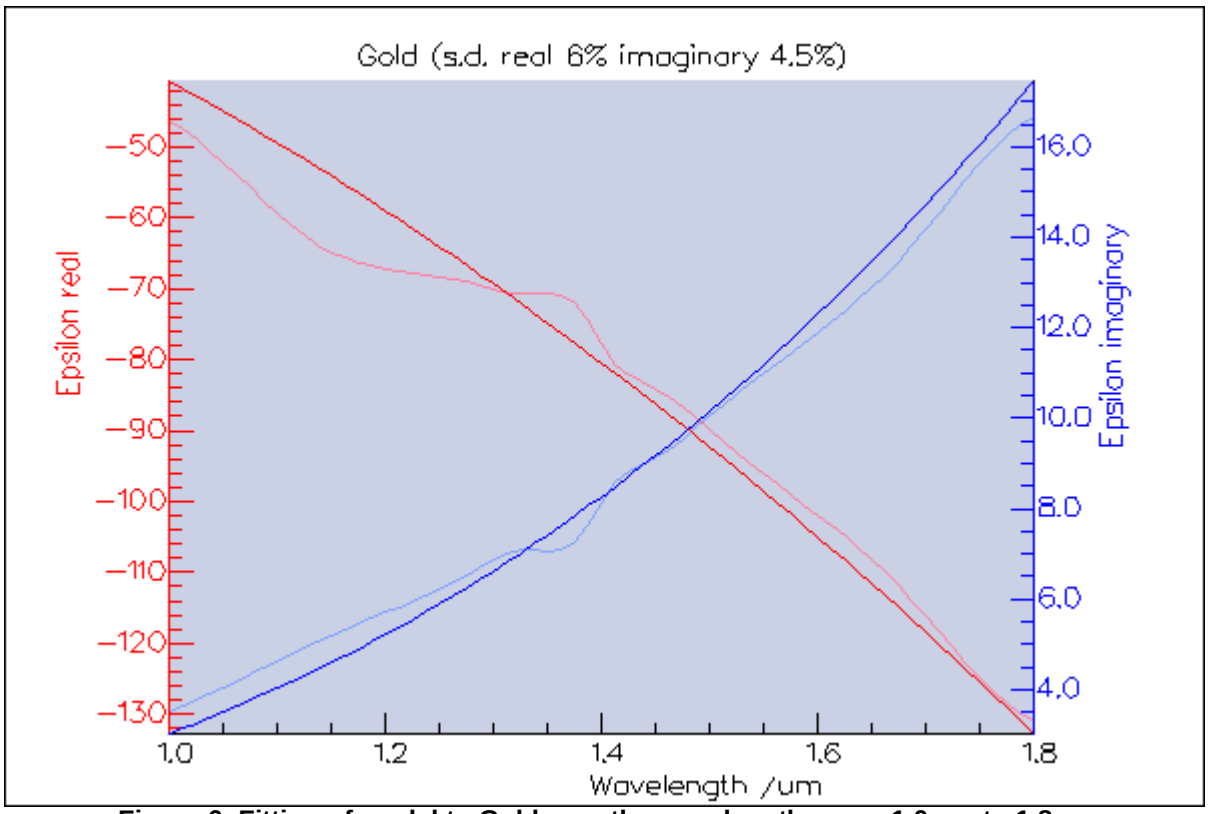

Figure 6: Fitting of model to Gold over the wavelength range 1.0 um to 1.8 um

The fit is now accurate to 6% in the real index and 4.5% in the imaginary index.

When the materials database is being used then it is not necessary to set the excitor wavelength for each calculation and a single OmniSim calculation can generate all the required wavelength information. Figure 7 shows a comparison between OmniSim and FIMMWAVE when the model has been fitted over the wavelength range 1 um to 1.8 um and from 1.4 um to 1.8 um

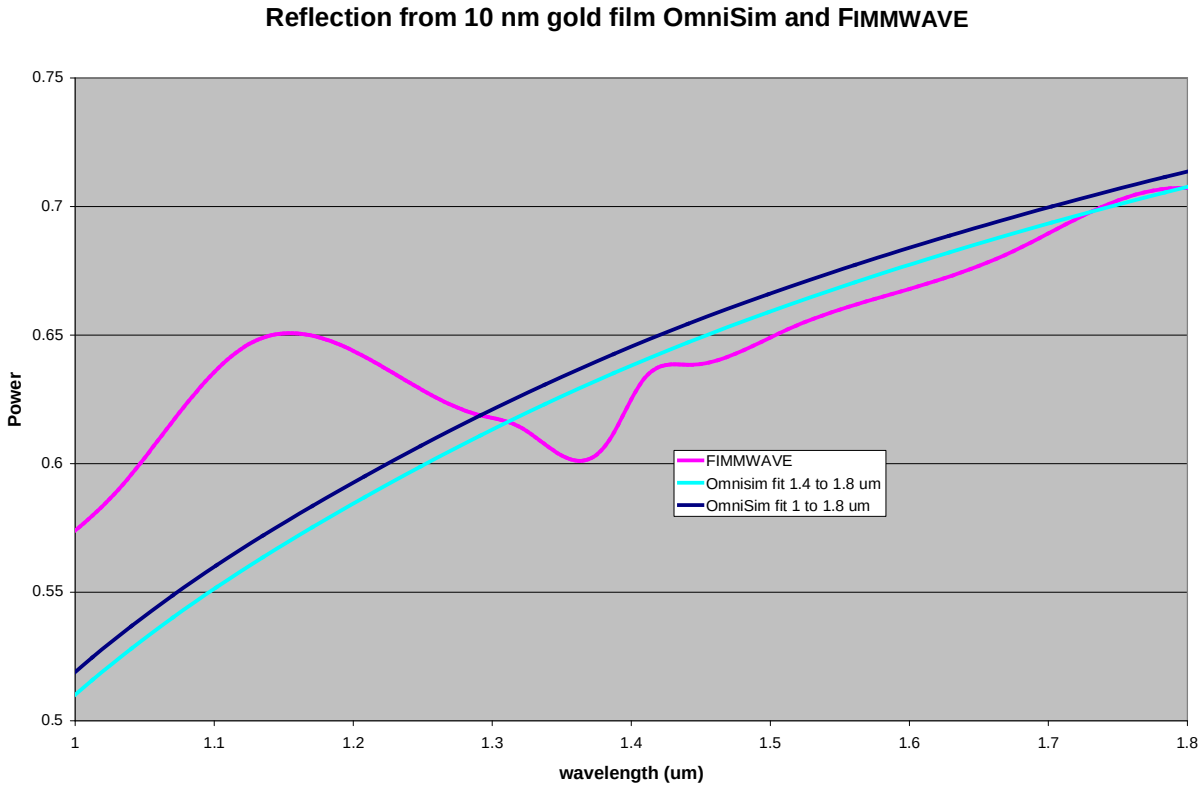

Figure 7: Comparison between OmniSim and FIMMWAVE for 10 nm gold film

There is moderate agreement, which improves over the range 1.4um to 1.8 um if the model is only fitted from 1.4 um to 1.8 um.

1.2.3. Test 3

In this test Tungsten has also been used figure 8 shows the fit from 0.4 um to 1.8 um, because resonance are present then a better fit for tungsten is obtained if the fit fully includes the resonances.

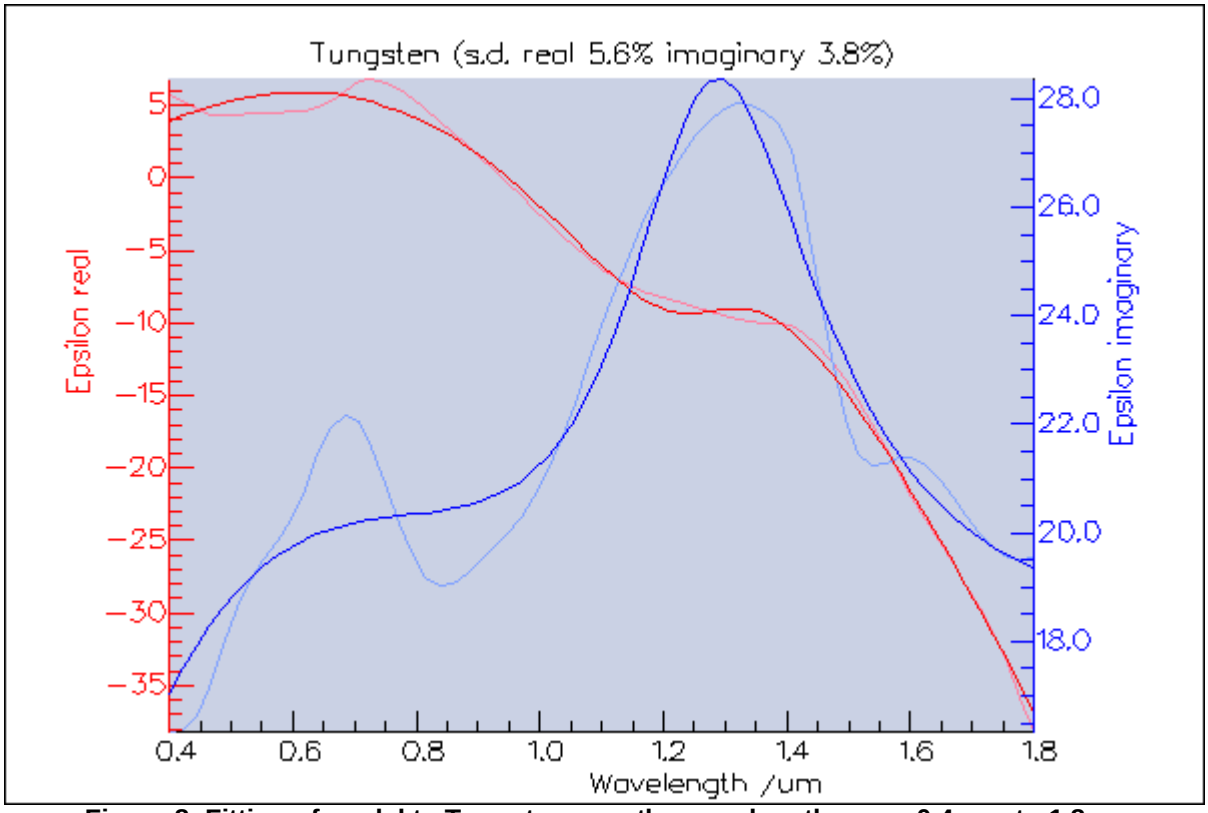

Figure 8: Fitting of model to Tungsten over the wavelength range 0.4 um to 1.8 um

Figure 9 shows the comparison between OmnSim and FIMMWAVE for a 100 nm thick tungsten film.

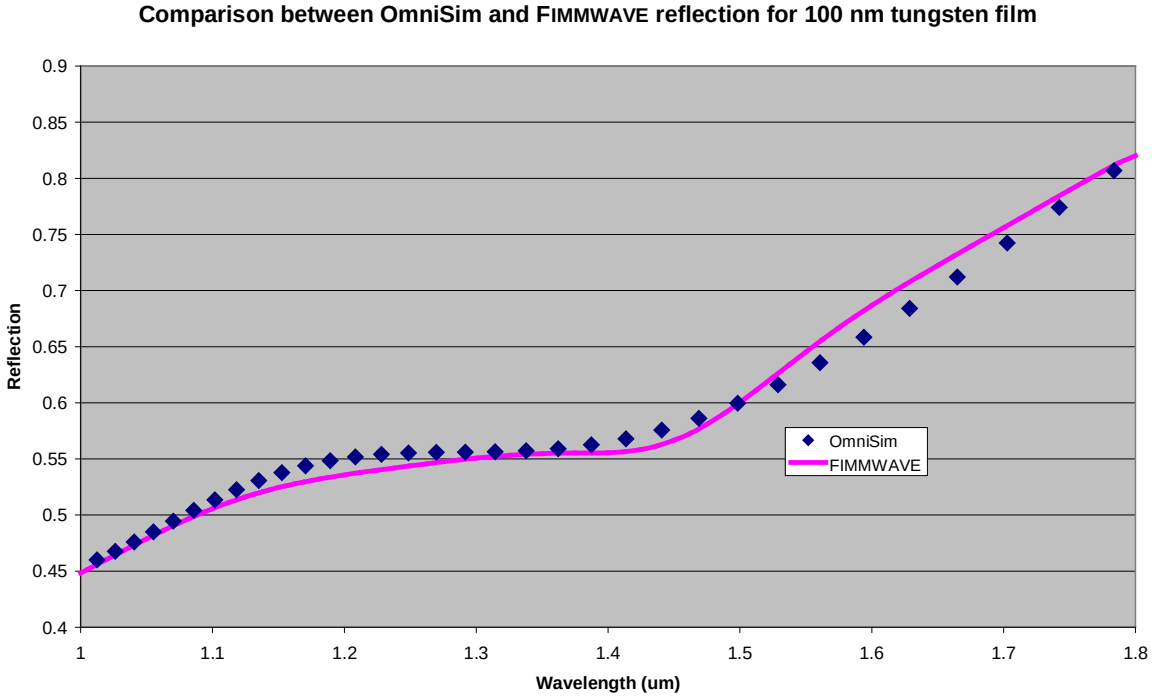

Figure 9: Comparison between OmniSim and FIMMWAVE for Tungsten

The agreement between OmniSim and FIMMWAVE is good over the entire wavelength range.

1.2.4. Test 4

In this test aluminium has been used as the metal and the model has been fitted from 0.4 um to 1.6 um. Figure 10 shows the fit

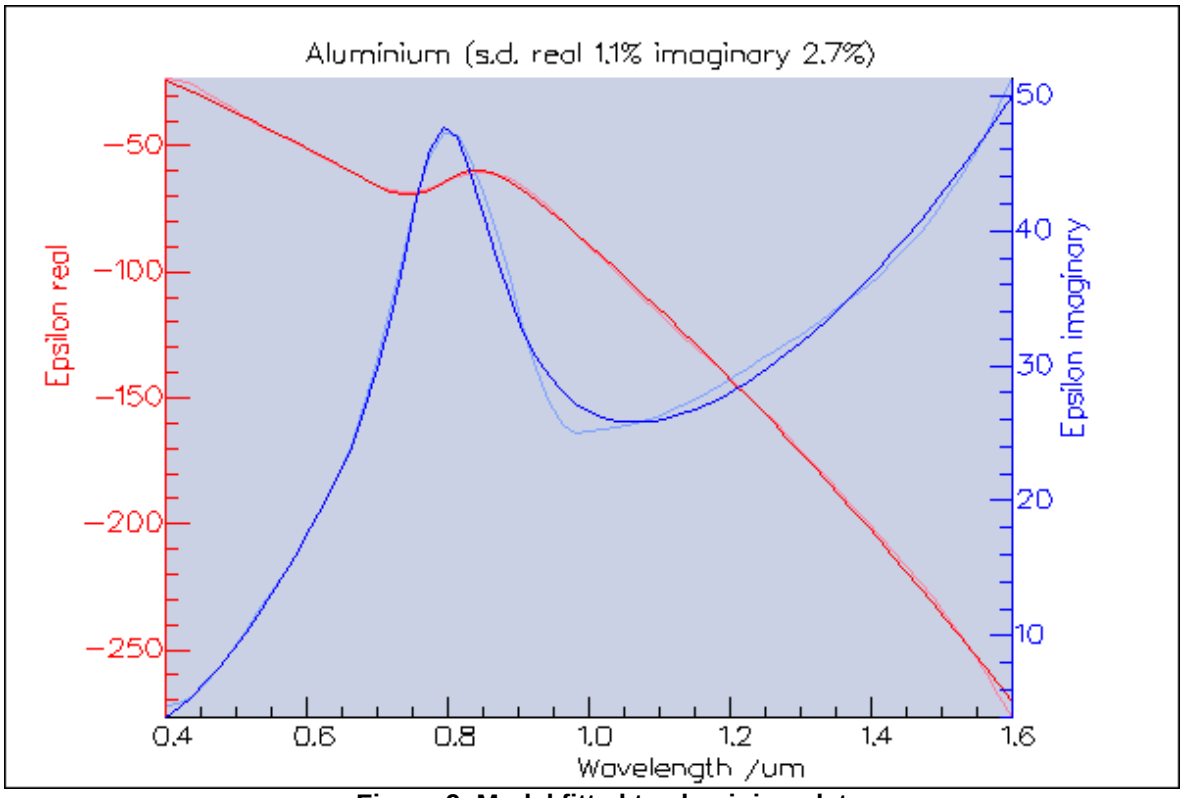

Figure 9: Model fitted to aluminium data

The results of the comparison which are shown in figure 10 show excellent agreement between FIMMWAVE and OmniSim. To achieve this result the aluminium film had to be positioned so that the boundaries were aligned with a grid boundary. Figure 11 shows the effect when the film boundary was midway between two grid points.

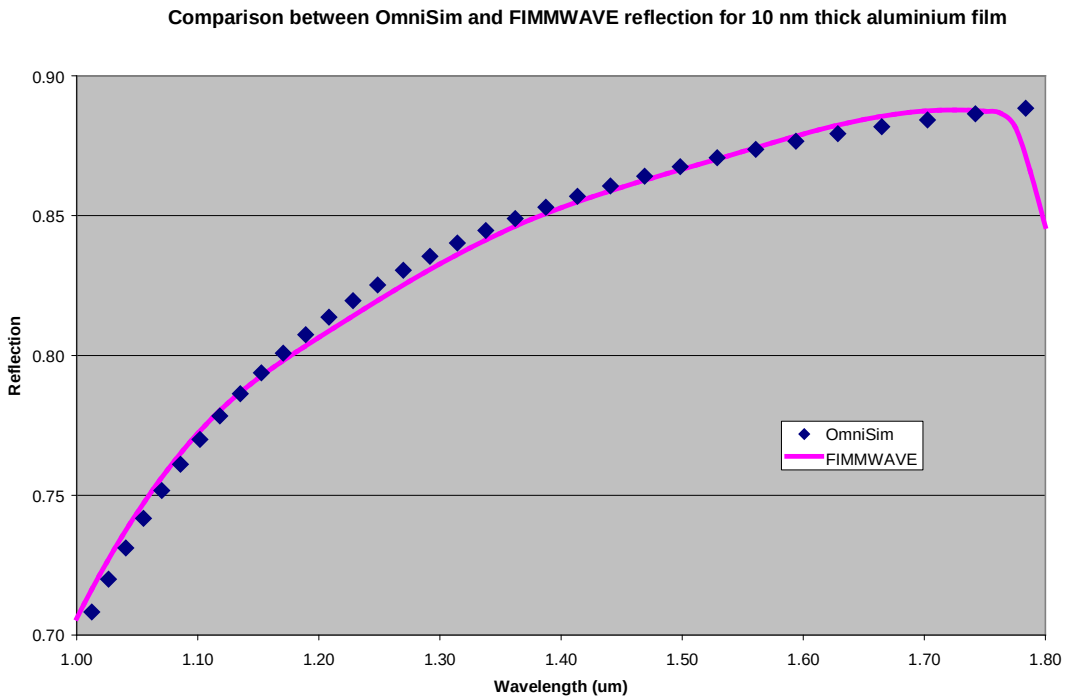

Figure 10: Results for 10 nm thick Aluminium film –film boundary aligned with grid

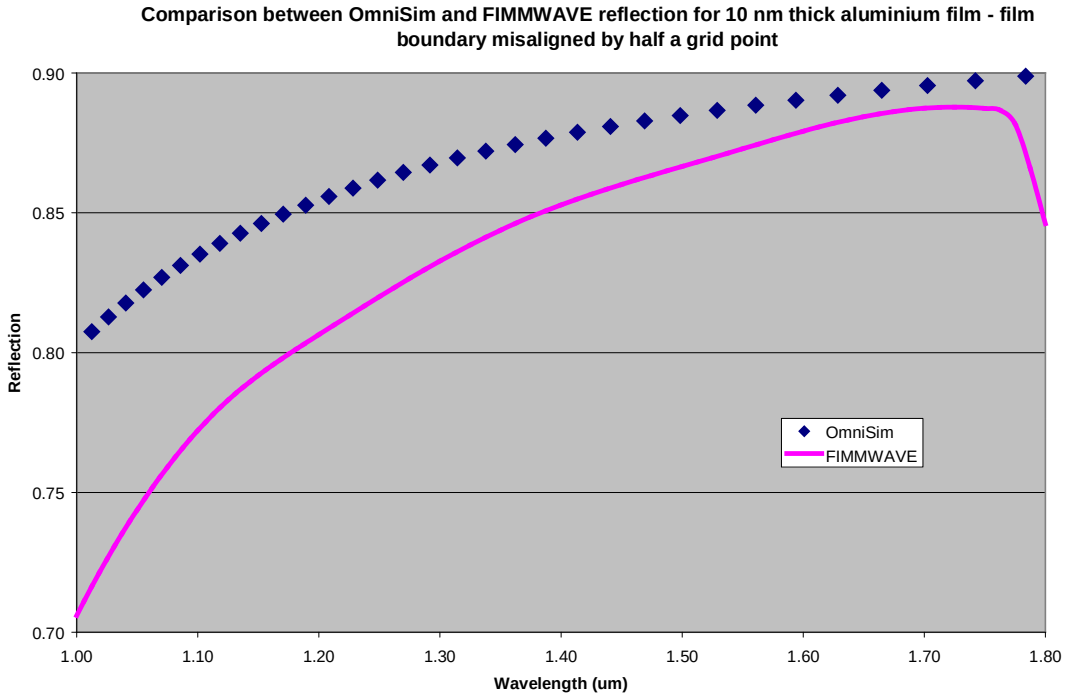

Figure 11: Results for 10 nm thick Aluminium film –film boundary misaligned with grid

1.2.5. Test 5

In this test nickel has been used, the fit and the results are shown in figures 11 and 12 and both show excellent agreement.

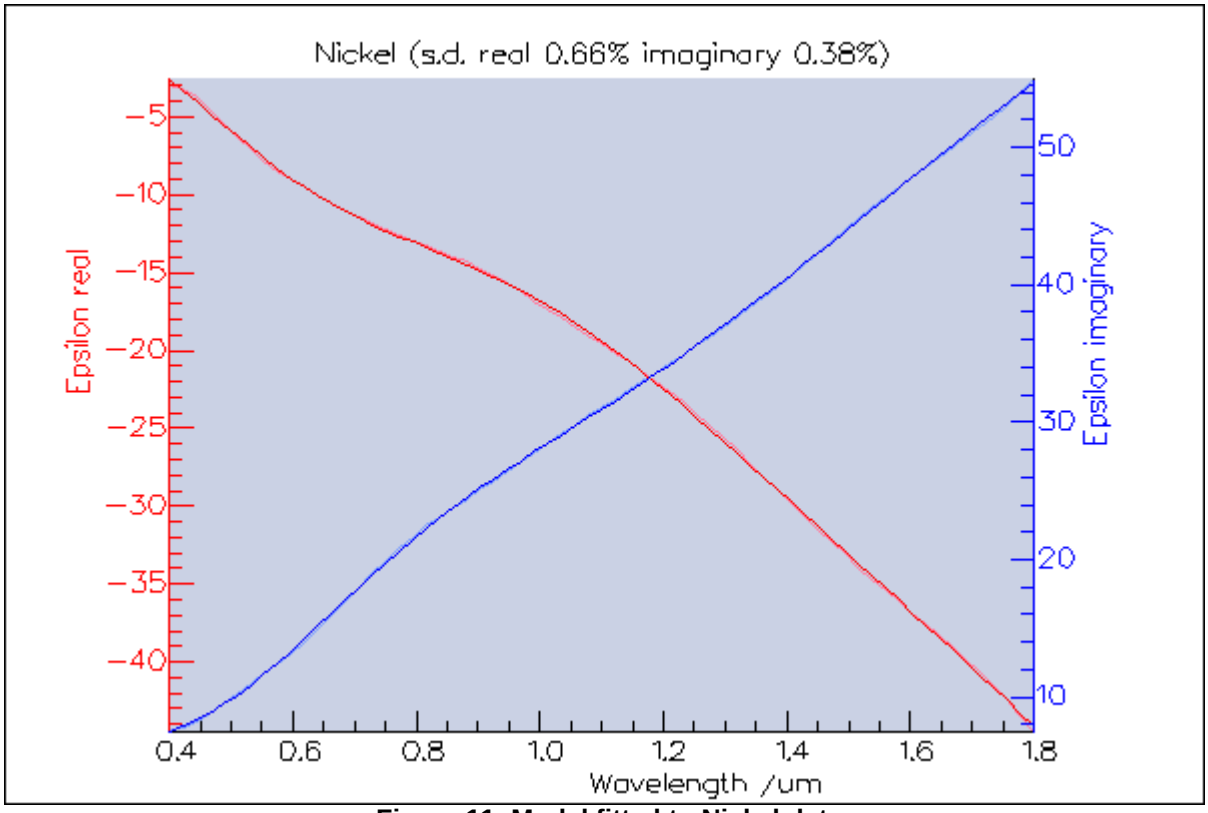

Figure 11: Model fitted to Nickel data

Comparison between OmniSim and FIMMWAVE reflection for 40 nm thick nickel film

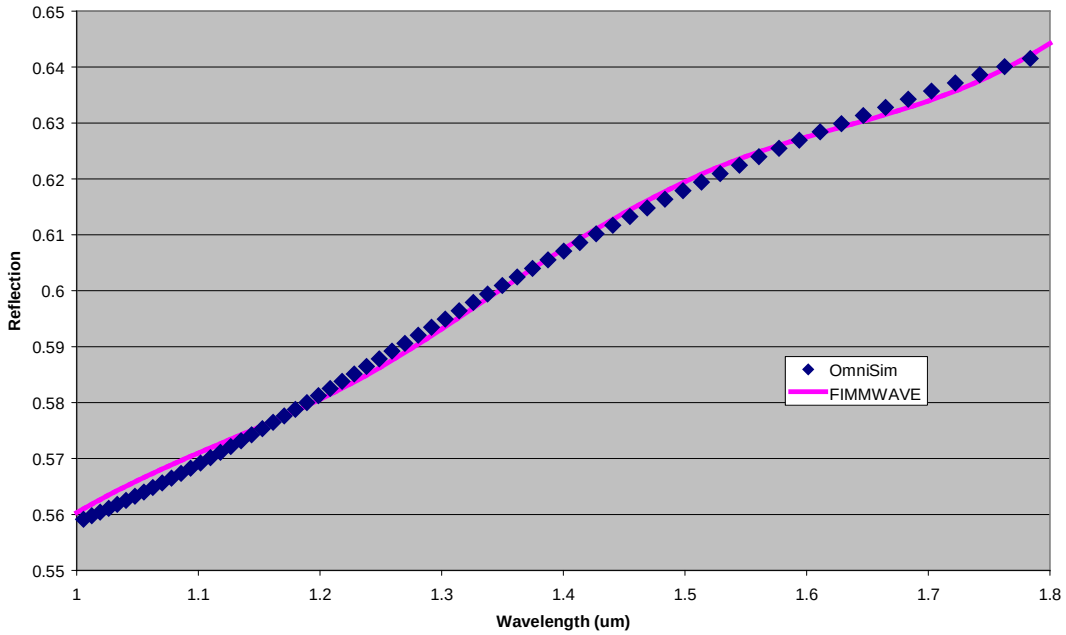

Figure 12: Results for 40 nm thick Nickel film

1.2.6. Test 6

In this test a Fabry Perot resonator was created by having two metallic mirrors separated by a 4 um air gap. The device is shown schematically in figure 13.

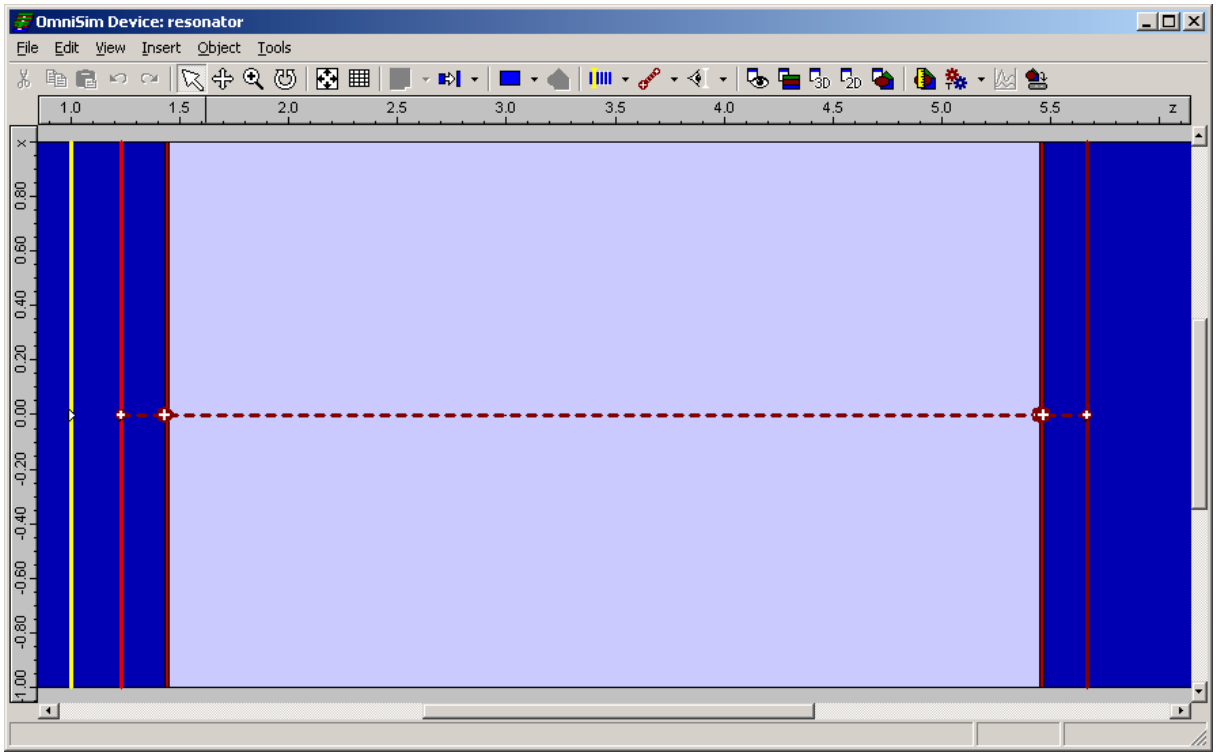

Figure 13: Schematic of resonator

The transmission of the resonator was calculated for gold thicknesses of 10 nm, 20 nm and 40 nm . In addition OmniSim can calculate the phase of the output field which can then be used to determine the group delay of the resonator. The group delay is the change of phase with angular frequency (ω) and can be rewritten as

$$\tau_g = \frac{\lambda^2}{2*\pi*c}\frac{d\phi}{d\lambda}$$ where c=speed of light

Figures 14 to 19 show the transmission and group delay for the three different thicknesses of gold. Increasing the thickness of the gold increases the reflectivity of the mirrors which increases the Q of the cavity. In all of these test there is excellent agreement between OmniSim and FIMMWAVE, in the peak wavelength, the peak width, the peak transmission and also the group delay.

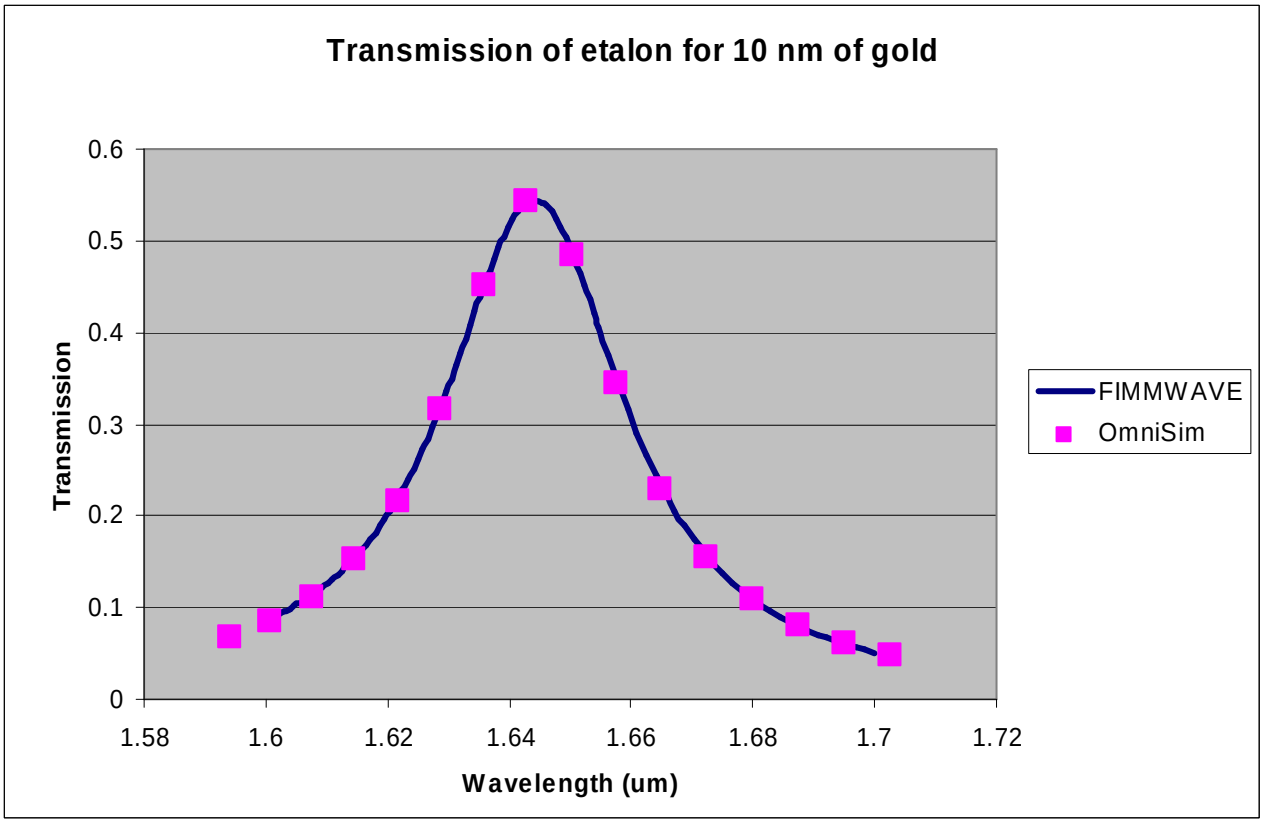

Figure 14: Transmission of etalon with 10 nm gold mirror

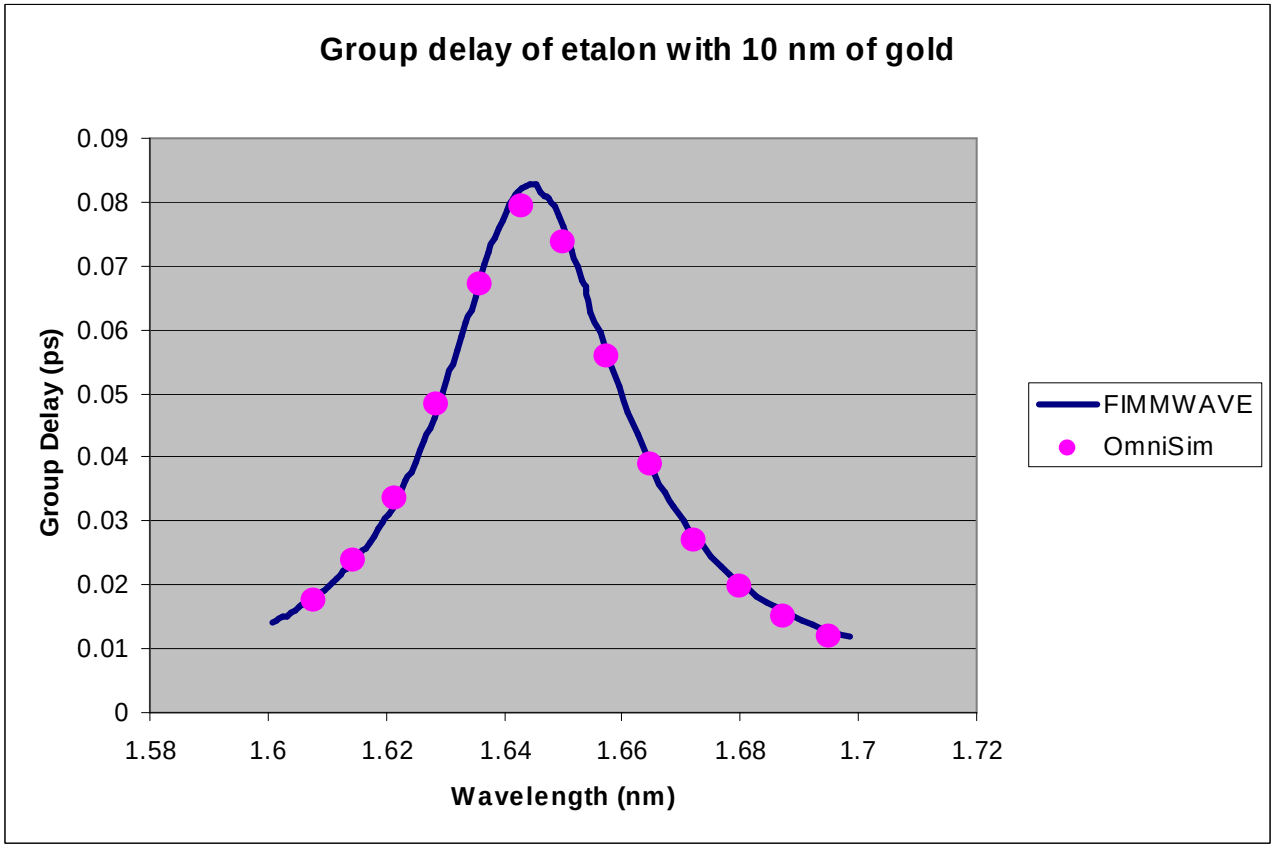

Figure 15: Group Delay of etalon with 10 nm gold mirror

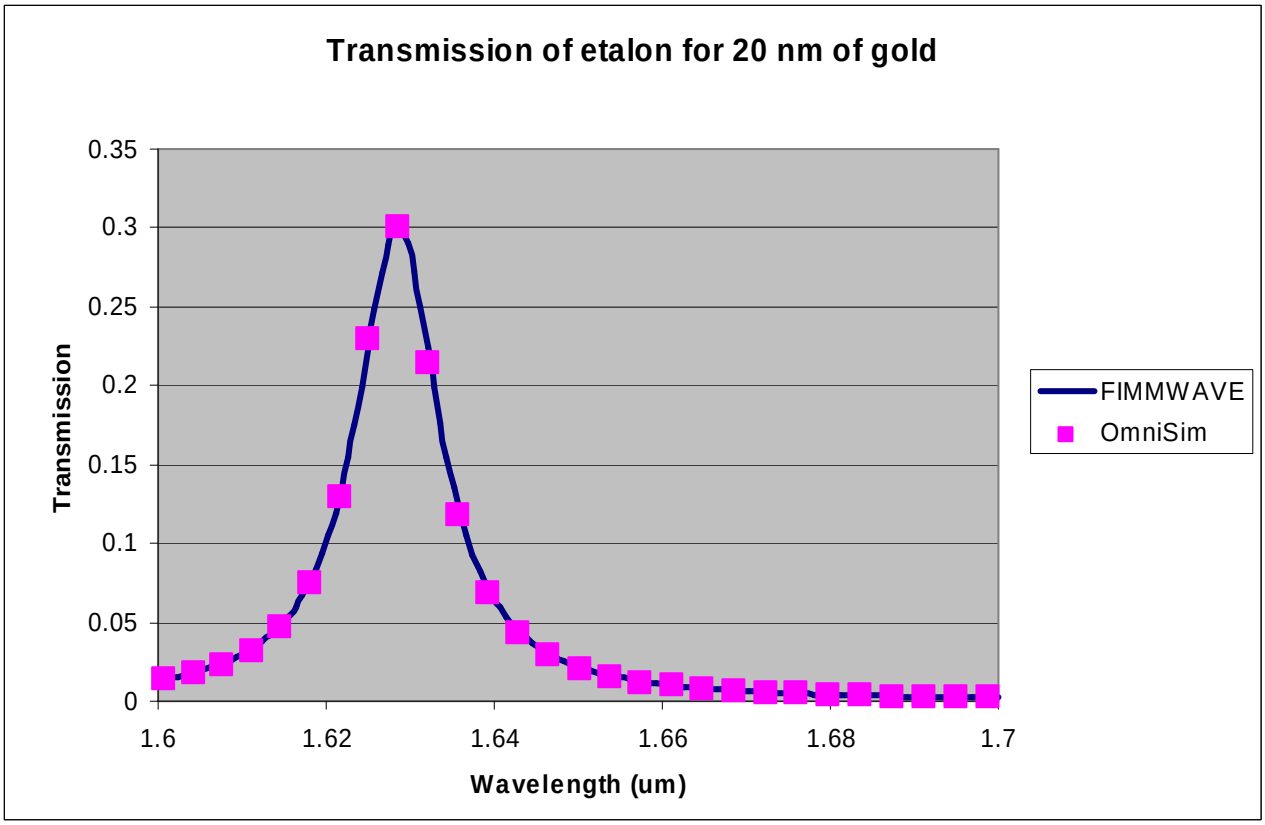

Figure 16: Transmission of etalon with 20 nm gold mirror

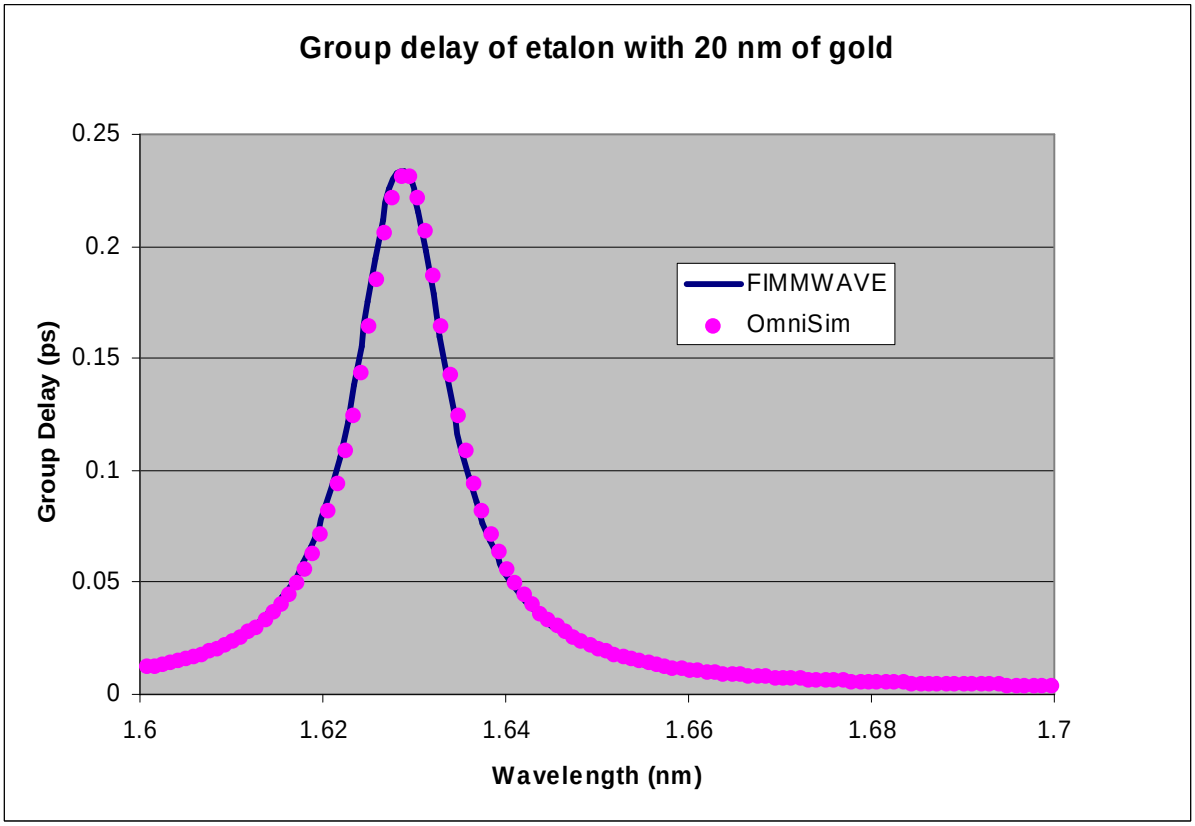

Figure 17: Group Delay of etalon with 20 nm gold mirror

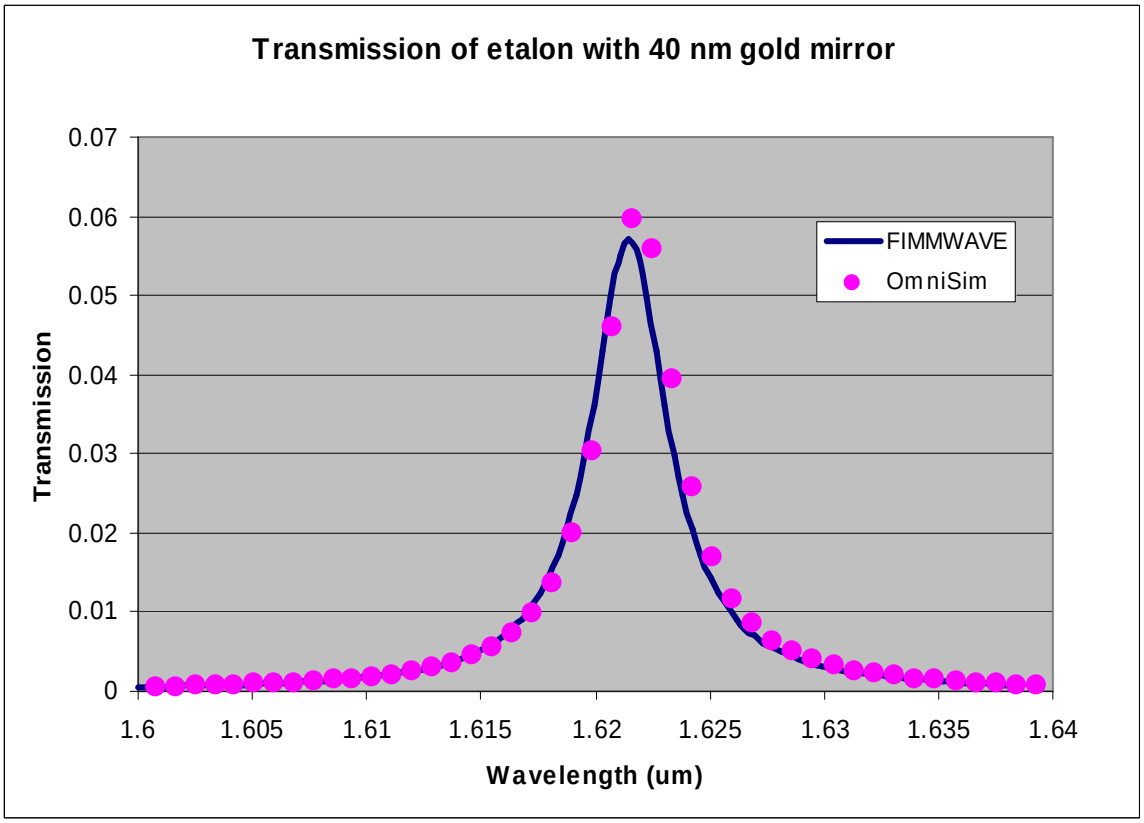

Figure 17: Transmission of etalon with 40 nm gold mirror

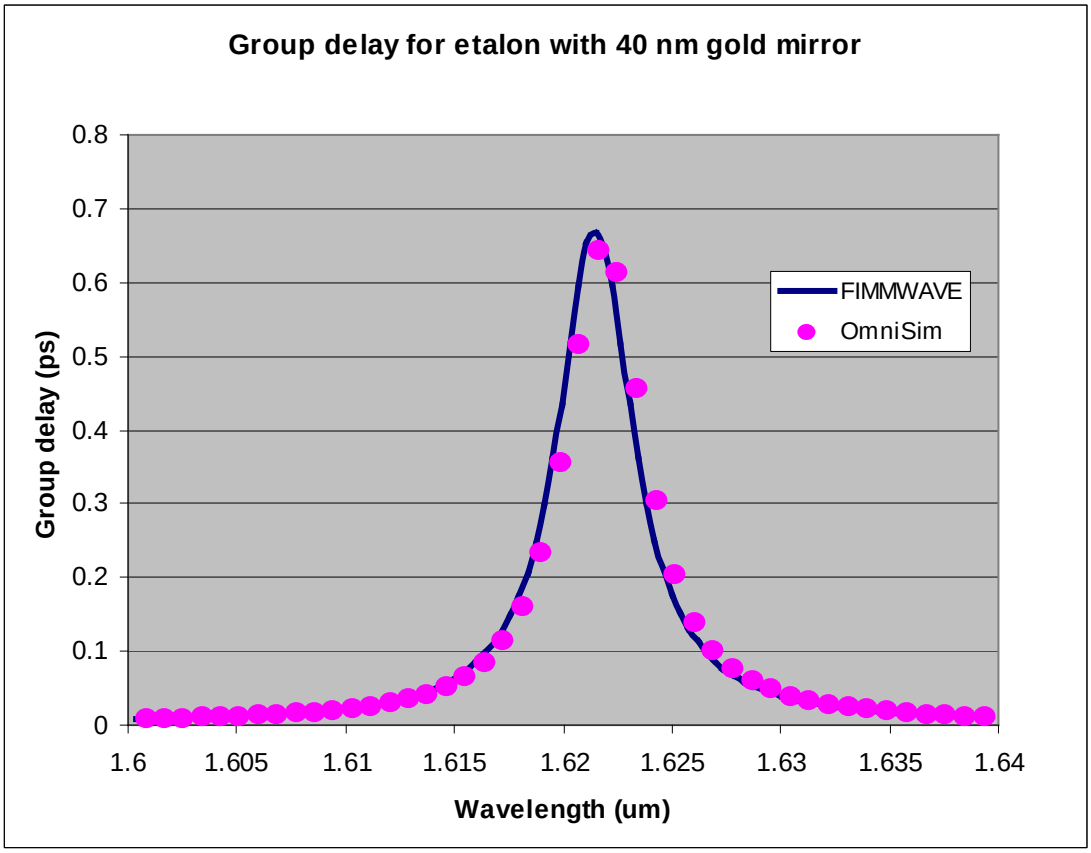

Figure 18: Group delay of etalon with 40 nm gold mirror

Conclusions

Test 1 demonstrated that for a layer with a fixed real and imaginary refractive index, there is excellent agreement between the transmission obtained from OmniSim and that from FIMMWAVE. There is a small error that is due to reflections from the PMLs.

Test 2-6 demonstrated that the fitting process used by OmniSim gives a good match to the transmission of a range of metals. The agreement between OmniSim and FIMMWAVE is largely determined by how accurately the model fits the material data.

Test 6 demonstrated that the transmission of an etalon is in excellent agreement and that there is also excellent agreement with the phase response, enabling the group delay to be calculated.