Using the S^4 software to optimise the design process of reflective epsilon-near-zero metasurfaces

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Introduction and Aims

Epsilon-near-zero (ENZ) metasurfaces have a great potential to provide a promising alleyway for the future of nonlinear optics due to their unique and curious properties, helping to enhance and improve optical technologies, such as fibre optic cables. However, the current design process for these surfaces is slowed down by the accurate but time consuming finite-difference time-domain (FDTD) method of simulation. By contrast, the Fourier Modal Method (FMM), while less accurate, simulates electromagnetic interactions much faster than the FDTD method, One such software that employs FMM is S^4, designed to solve Maxwell's equations in layered periodic structures[1]. Its use could greatly increase the production rate of such surfaces, and thus make their use more widespread. In the investigation, the software is tested for its simulation of reflection spectra from ENZ metasurfaces in comparison to corresponding FDTD simulations. The design is then optimised for high reflectivity in optical fibres.

What are ENZ metasurfaces?

An **epsilon-near-zero** material is one whose **real part of the permittivity is close to or crosses zero** within a certain wavelength range while the imaginary part remains finite, and which exhibit a **strong nonlinear response**[2]. Light in these materials exhibits interesting properties, including the phase velocity of the wave tending to infinity, and slow modulations in the amplitude of the wave[3].

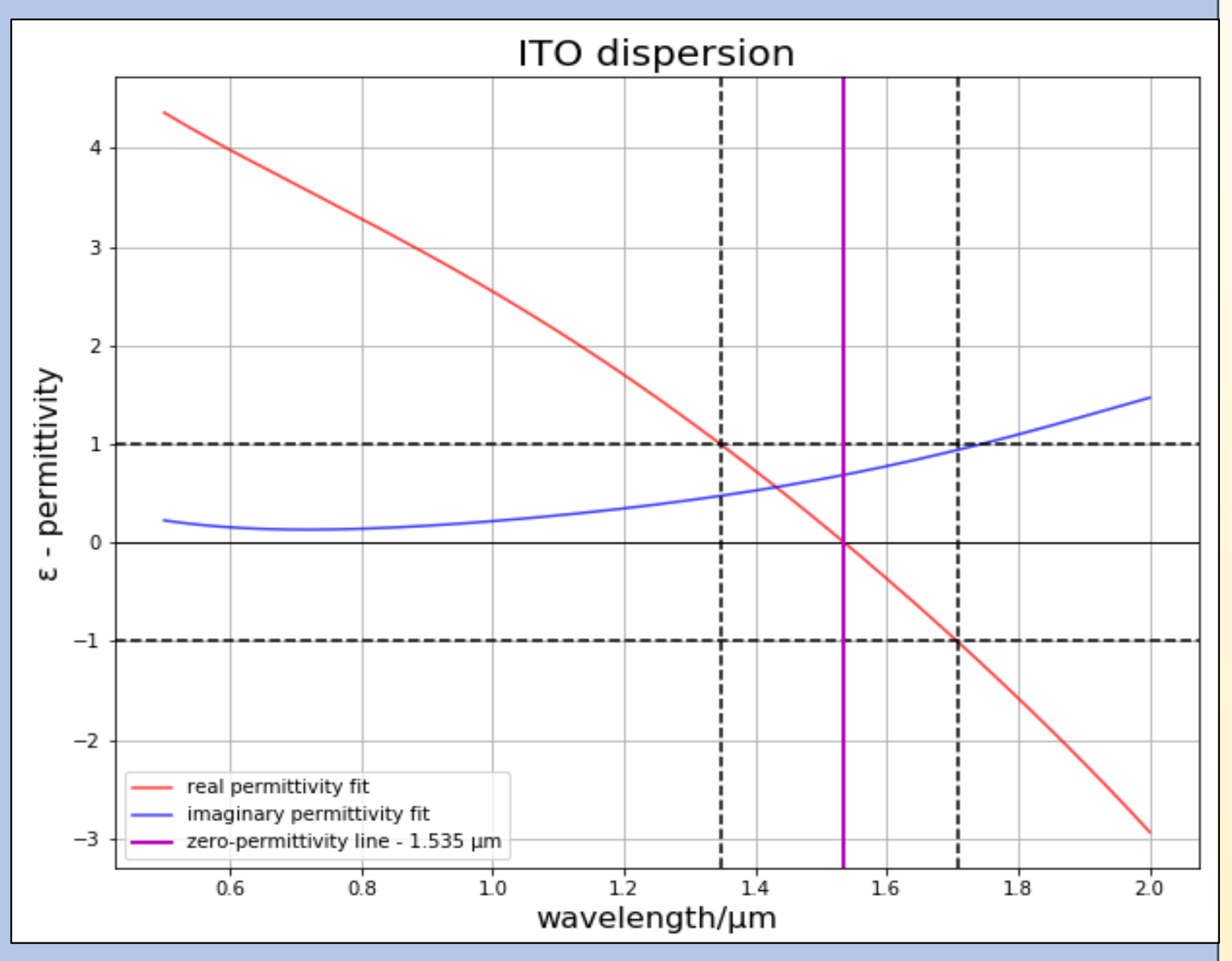

Figure 1: A plot of the dispersion of an ENZ material (indium tin oxide – ITO). The red and blue curves represent the real and imaginary permittivities respectively, while the purple line indicates the wavelength at which the former is equal to zero.

Metasurfaces are planar surfaces of subwavelength thickness containing in-plane features, displaying **inhomogeneous phase distribution for electromagnetic waves** incident on them[4].

This is usually achieved by optical antennae placed periodically in arrays on the surface of some spacer. The shape and orientation of each antenna determine how it interacts with light and the phase that it imprints, allowing for better optical control, and thus for a variety of designs for different purposes

Figure 2: An example of a metasurface made from a nanoantenna array, creating negative refraction

Image adapted from Birck Nanotechnology Center, Purdue University

The S^4 software and method

The S^4 software is fronted by the Lua programming language, and this was used instead of the Python extension since the software is predisposed for its use. Here, the base unit length was defined as one micron, and the primary wave as normally incident an p-polarised (in the software, this is defined as polarisation along the x-axis).

Each simulation began with a standard block of code defining the lattice (the simulation region), the number of Fourier expansions to be used, the materials used, and the surface structure. Polynomial fits to the materials' dispersions were obtained in Python, which were then manually translated into Lua in the form of arrays to form polynomial functions (as Lua has no automatic "array" command). These were then coded into a "for" loop to provide the correct value of material permittivities for each wavelength iteration.

Indium tin oxide (ITO) was used in the investigation as the ENZ material, and a gold antenna and back-reflector were used to produce the reflection spectra.

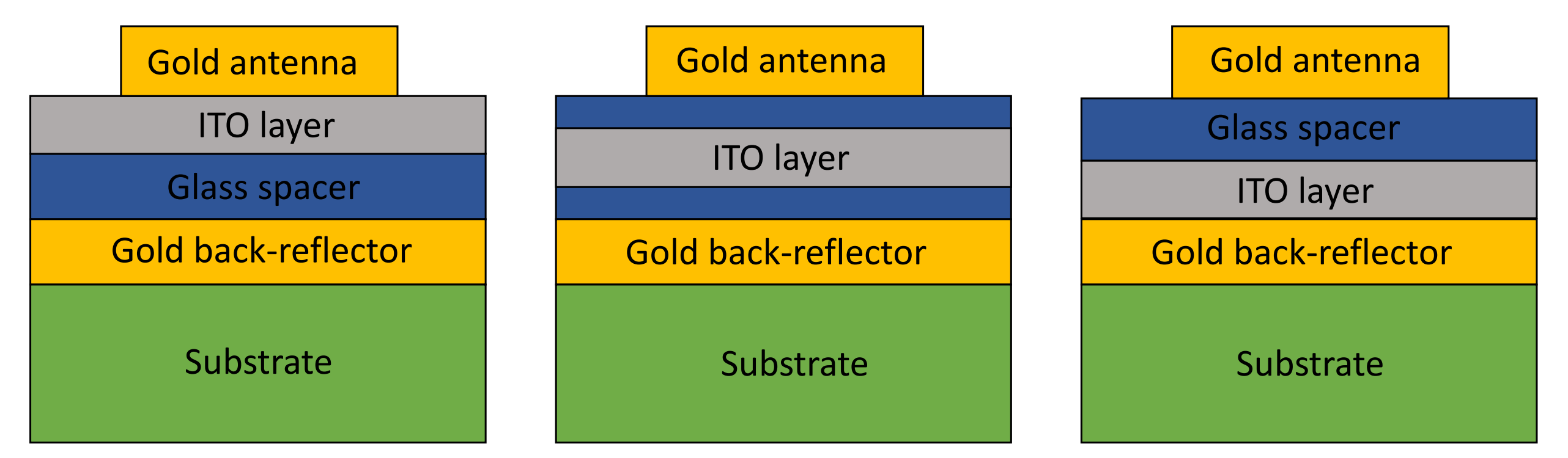

Figure 3: A schematic of the surfaces used for simulation. In this example, we test how the position of the ITO layer affects the reflectivity of the surface

References

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[4] Q. He, S. Sun, S. Xiao, L. Zhou, *"High Efficiency Metasurfaces: Principles, Realizations, and Applications*", Advanced Optical Materials, **6**, 1800415 (2018)

Results

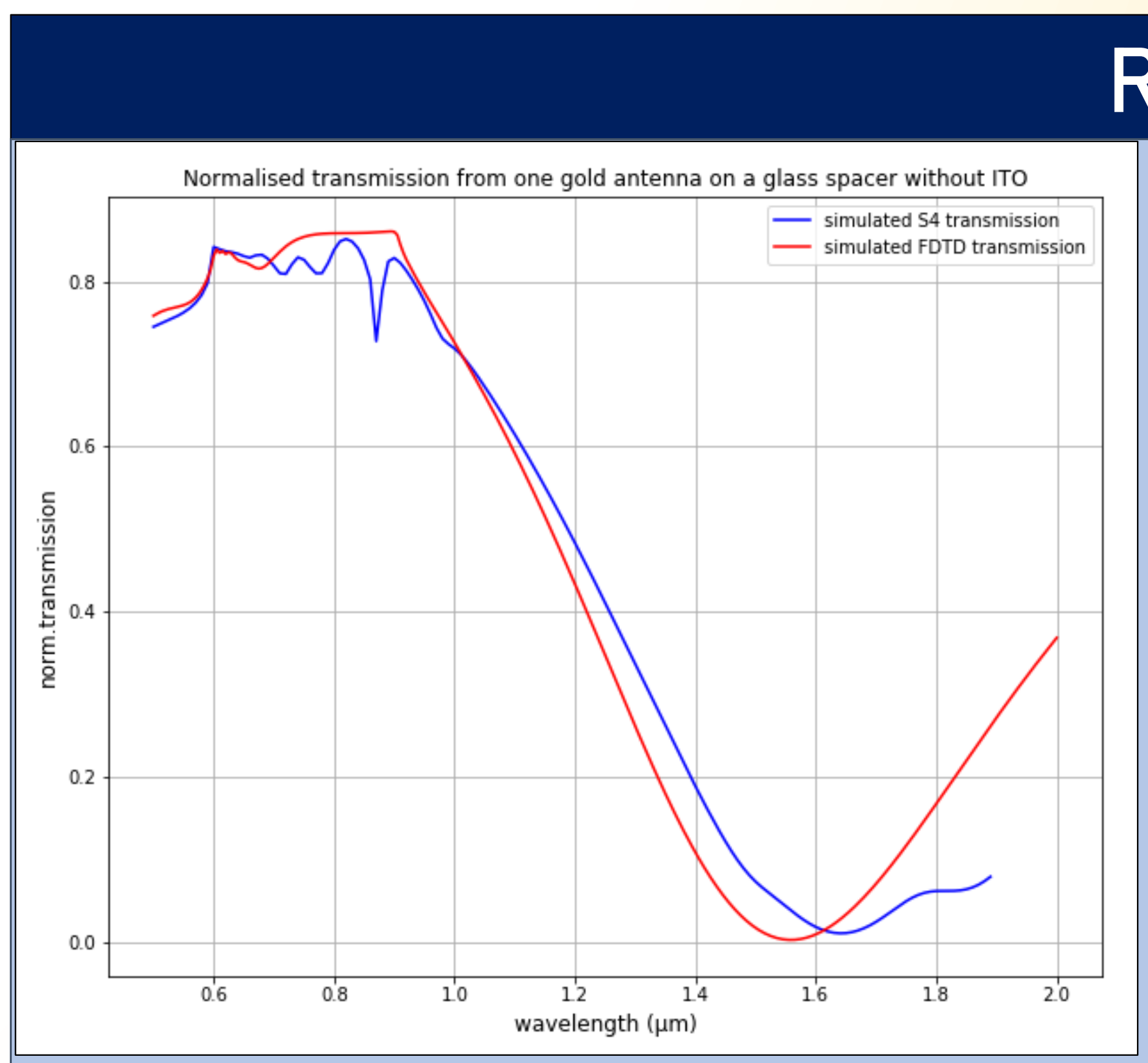

Figure 4: Normalised transmission from one gold antenna on a glass spacer, with FDTD and S^4 simulations shown by the red and blue curve respectively.

1) A control simulation was made to test how accurately S^4 could simulate the transmission from simple surfaces containing no ITO layer as shown in Figure 4. The FDTD curve and its characteristic features were recreated to a good degree of accuracy.

2) The simulation was run with the ITO layer in place above the glass spacer (Figure 5, top). Although the peaks and amplitudes are offset slightly from the FDTD curve (in blue), **the error margin is small**, and this is a good approximation of the reflection spectrum **considering the short simulation time** (approximately an hour). Additionally, it was found that placing the ITO layer underneath the glass spacer yielded more favourable results for reflection (Figure 5, bottom). Again, the characteristic features of the FDTD curve (in black) are reproduced, but the amplitude of the peaks is greater than for the preceding simulation. Already, this lets us deduce that placing the ITO layer nearer the back-reflector is a better design choice for reflective metasurfaces.

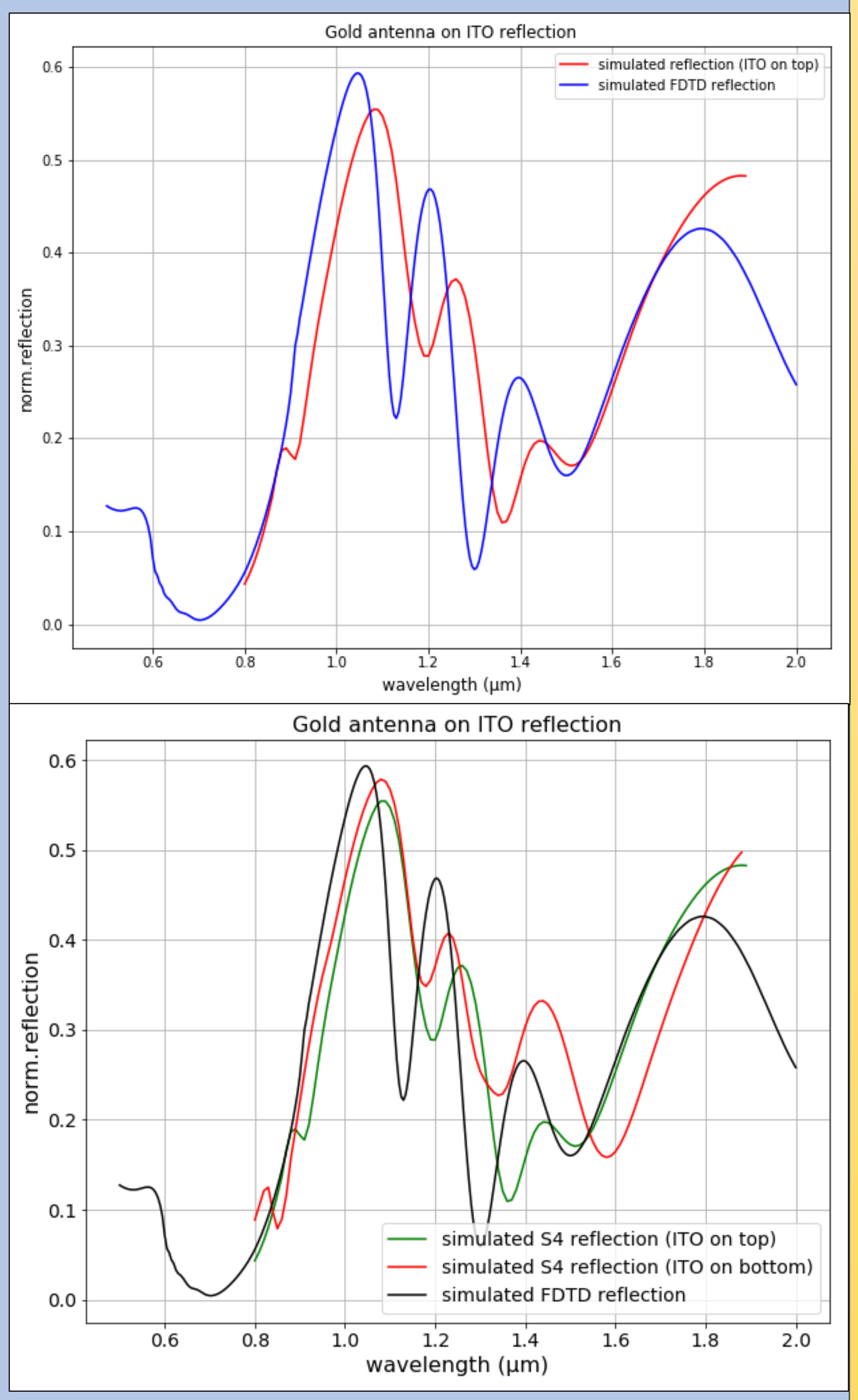

Figure 5: Normalised reflection from the surface with the ITO layer in place; the bottom graph additionally shows the reflection spectrum with the ITO layer underneath the glass spacer

Figure 6: Normalised reflection from the unmodified (blue) and modified (red) surfaces in the S^4 simulation.

3) Modifications to the antenna and surface dimensions were made to optimise its use for optical fibres operating at around the 1550 nm wavelength. To be effective, the normalised amplitude of the peak must be 0.8 or above. As seen in Figure 6, this was well approximated by the software in a relatively short time. To achieve this reflection, the simulation region was reduced in the **y-axis from 600 nm to 500 nm**, and the antenna dimensions as well as the simulation region were lengthened in the **x-axis from 420 nm to 670 nm**, and **from 600 nm to 900 nm** respectively. The modified parameters can be entered into an FDTD simulation for an accurate check and to make further improvements.

Conclusion

Overall, this investigation has successfully shown that the S^4 software can be used as a fast-approach method of simulating reflection spectra of ENZ metasurfaces. The software simulates the FDTD results to a good degree of accuracy in a considerably shorter time, making it a useful tool for early stage design processes of these surfaces. Moreover, its fast simulation time allows for parameter modifications to be made quicker, thus making it possible to produce a wider range of designs for a variety of purposes at a greater rate. Although these would still have to be checked with the FDTD simulations for greater accuracy, the use of S^4 will greatly accelerate the design process of ENZ metasurfaces, ultimately making them more accessible in various fields and industries.

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