Computation Simulation of Gold Core/Shell Nanostructures for Near Field Transducers in Heat Assisted Magnetic Recording

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Introduction:

Localised surface plasmon resonances (LSPR) are highly geometry dependant collective electron oscillations in metallic nanostructures that are excited by radiation. At the resonant wavelength, a greatly enhanced E-field is expressed in the near-field region around the nanoparticle. This phenomenon shows amazing promise as a coupling mechanism for sub-diffraction limited confinement of optical energy for Heat Assisted Magnetic Recording (HAMR)[1].

An unfortunate result of this confinement is a thermal energy build up in the nanoparticle (Near Field Transducer) itself which, among other detrimental effects, can result in antenna deformation and hence alteration of the geometry dependant resonance condition.

This study examines the effect of shell materials and thickness on the resonance position and thermal energy distribution of a spherical gold nanoparticle with the aim of reducing heating in the gold sphere while limiting the wavelength shift of the resonance.

Computational Methods:

The model geometry is demonstrated in Figure 1. Plane polarised radiation propagates from a port at the top of the model and is incident on the nanostructure which is surrounded by air. Underneath is a surface within the air domain used for normalised average power integrals, and finally a PML which is half the maximum wavelength in height. Floquet boundary conditions are applied to the sides of the model to impose symmetry on the solutions while the period is set to 800nm to prevent periodic effects. The RF Module of COMSOL Multiphysics® the equation:

$$\nabla \times (\nabla \times \mathbf{E}) - k_0 \varepsilon_r \mathbf{E} = 0$$

Is solved for the Electric field vector (**E**) where k_0 is the vacuum wavelength and ε_r is the relative permeability. The relative permeabilities of the nanoparticle materials are governed by frequency dependant complex refractive indices, which are evaluated using an interpolation of the Johnson and Christy data[2] for gold and silver, Palik data[3] for copper and from ellipsometry measurements of thin films of titanium nitride.

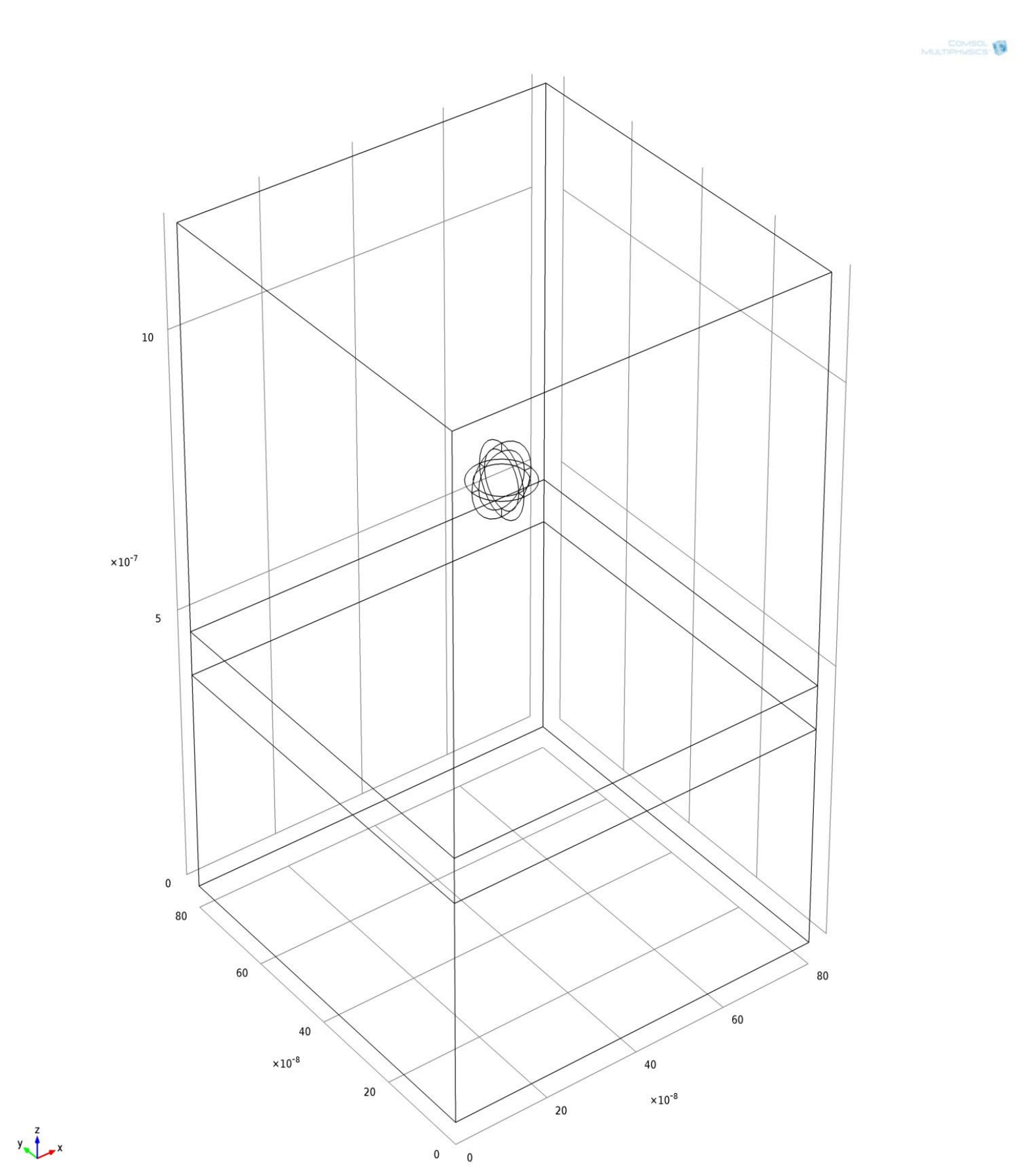

Figure 1. A wire frame diagram of the model geometry. The Uppermost domain is air containing the core/ shell nanostructure and a non-physical surface for power integration. The lower domain is a PML to attenuate transmitted radiation and prevent reflections

Using the air surface above the PML and a parametric sweep through wavelengths of 450nm to 800nm, power flow could integrated to evaluate the extinction spectra of the nanostructure for each value of shell thickness. This was confirmed using the S11 element of the scatter matrix i.e.

$$Extinction = -\log(1 - emw.S11)$$

Plots of the total dissipative power losses in the structure could then be taken and used as a proxy to describe the temperature of various regions in the structure and compare the effects of shell materials on the heating of an unclad gold sphere.

Results:

Figure 2a shows that the introduction of a shell layer of 5nm shifts the resonance peak no more than ~5nm towards the red end of the spectrum compared to an unclad 50nm radius gold sphere and the peak is un-shifted compared to a solid gold nanoparticle of equal size. The exception is a silver shell which shows signs of a slightly shifted but unresolved peak. Figure 2b shows the introduction of a 15nm shell layer introduces a shift of 10nm for copper and titanium nitride shells and a 5nm shift a silver shell compared to an unclad 50nm radius gold sphere. Compared to an equal sized gold particle the gold/silver structure is 5nm towards the blue and the gold/copper, titanium nitride structures are shifted 5nm towards the red.

References:

1. W. A. Challener et al, Heat-Assisted Magnetic Recording by a Near-Field Transducer with Efficient Optical Energy Transfer, Nature Photonics, 3, 2220-224 (2009)
2. P. Johnson and R. Christy, Optical constants of the Noble Metals, Phys. Rev. B, Volume, 4370-4379, (1972)
3. E. Palik, Handbook of Optical Constants of Solids ISBN 0-12-544420-6 (1985)

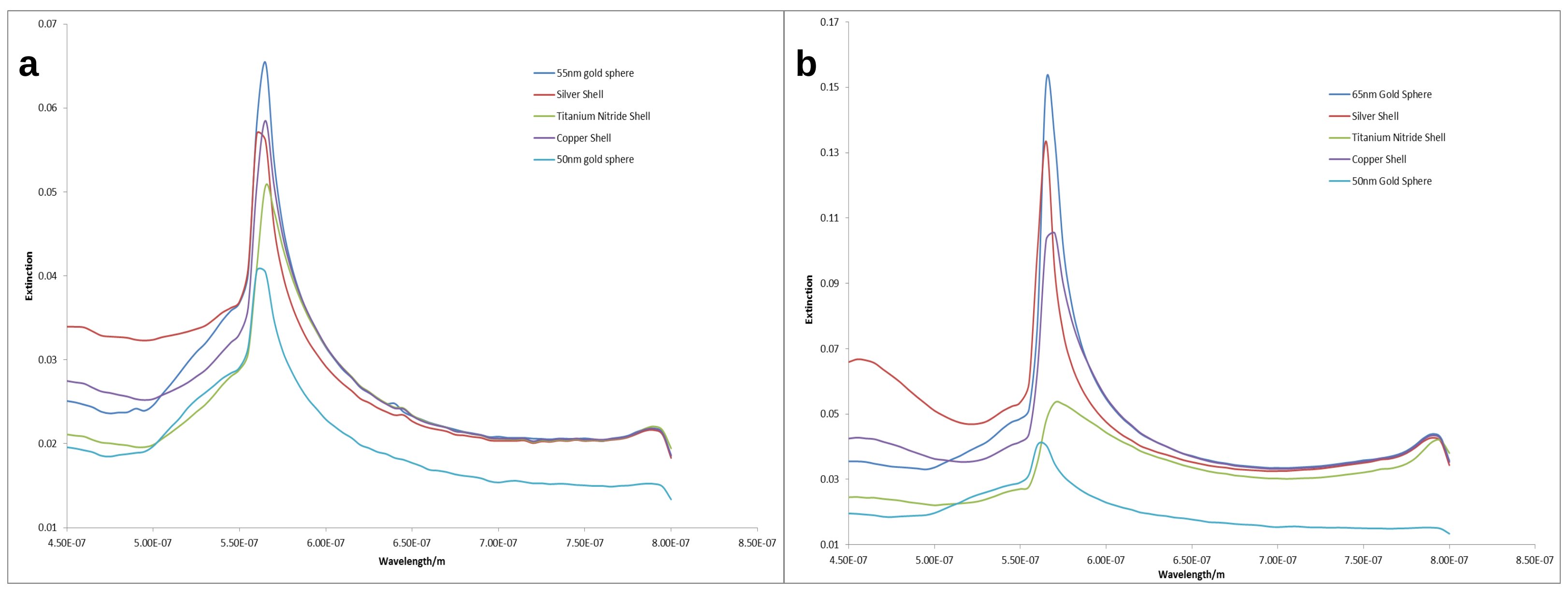

Figure 2a. Extinction spectra for 50nm radius gold cores with 5nm thick shell and unclad 50nm and 55nm radius gold spheres. Less than 5nm shifts observed in resonance location from the unclad resonance **2b** Extinction spectra for 50nm radius gold cores with 15nm thick shell and unclad 50nm and 65nm radius gold spheres. Shifts from resonance 5nm for silver and larger gold sphere, 10nm for Titanium nitride and copper.

The gold sphere experiences the greatest losses (and therefore greatest heating) at the top of the sphere closest to the port, a significant amount occurs at the sides perpendicular to the dipole resonance ie. The z-y plane.

The silver shell reduces the maximum power dissipation by 2 orders of magnitude and experiences more power loss in the z-x plane than the z-y plane, however the most intense heating occurs in the gold core as opposed to the silver shell.

In the case of copper the maximum magnitude of power loss is slightly increased over gold (< 1 order of magnitude) but is mainly focused at the top of the structure and to a lesser extent the z-y plane. Almost all of the power loss is confined to the copper shell.

The titanium nitride shell behaves as a heat dissipating dielectric, the maximum losses are largely unaffected but are mostly confined to the TiN shell. The resonance is observed to originate from the surface of the gold core, which leads to higher losses in the z-x plane than the z-y.

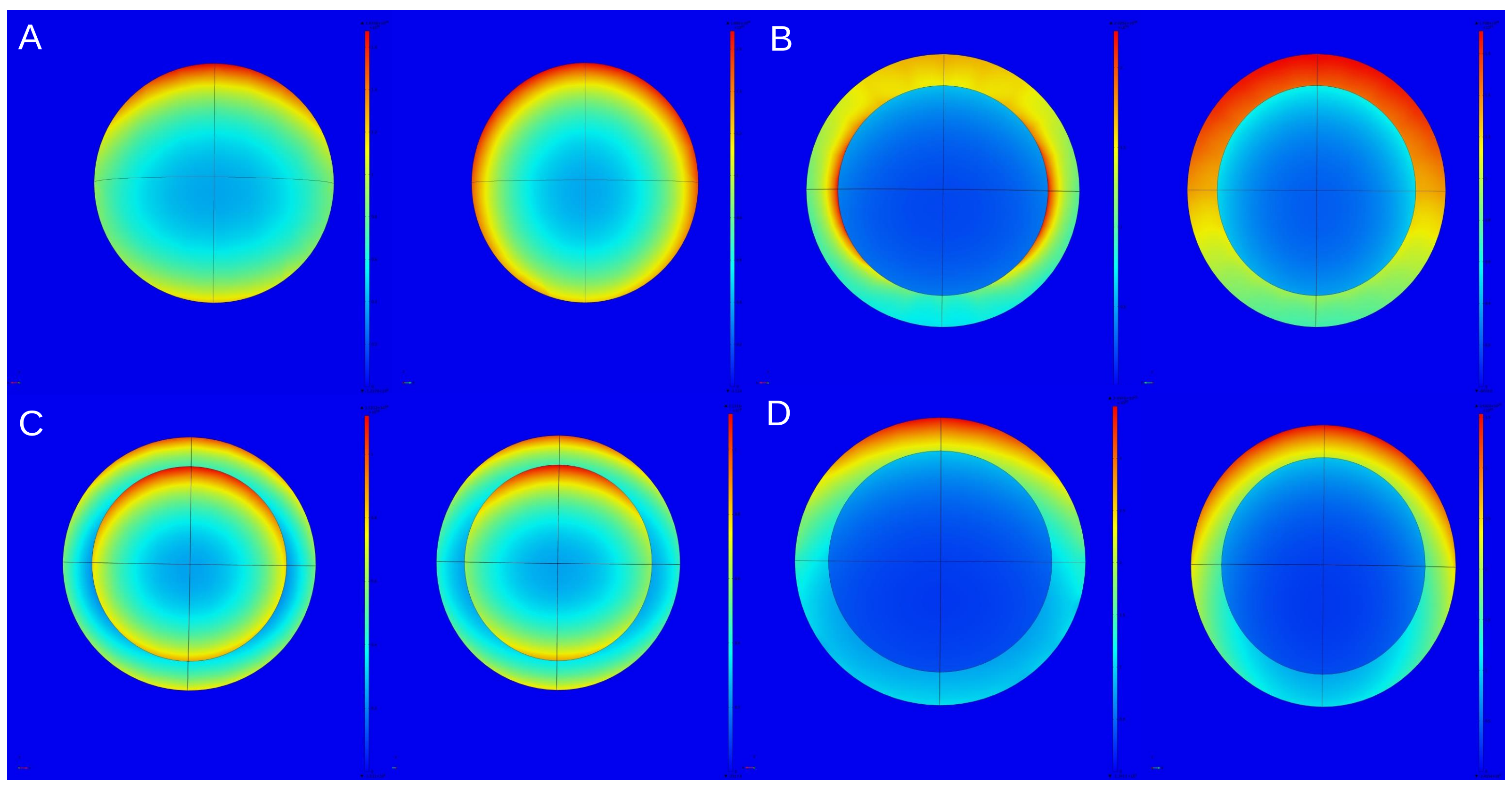

Figure 3 Dissipative power losses at resonance in z-x (left) and z-y (right) planes for **A)** 65nm gold sphere **B)** 50nm gold core with 15nm TiN shell **C)** 50nm gold core with 15nm Ag shell **D)** 50nm gold core with 50nm Cu shell.

Conclusions:

The addition of shell layers to spherical gold nanoparticles decreases the strength of the LSPR compared to pure gold particles of similar size, however the resonance is stronger than having the core with no shell.

With respect to reducing thermal build-up in the gold core, the addition of a silver shell is a poor choice since the majority of thermal energy is still localised within the core while titanium nitride and copper shells manage to confine major heating to the shell layer.

Titanium nitride shows less promise than Copper as a shell material in the context of HAMR because while the magnitude of the power losses is similar, the strength of the observed resonance is not. Therefore a similar temperature in the near-field transducer would be achieved for a lower coupling efficiency.

Copper proves the best shell material between the three, able to confine thermal build-up to the shell and produce a relatively strong resonance.

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